A6

PCT WORLD INTELLECTUAL PROPERTY ORGANIZATION
International Bureau

INTERNATIONAL APPLICATION PUBLISHED UNDER THE PATENT COOPERATION TREATY (PCT)

(51) International Patent Classification 5 :
A61K 39/00, 39/02, 39/12, 37/02, 35/14

A1

(11) International Publication Number: **WO 95/31997**

(43) International Publication Date: 30 November 1995 (30.11.95)

(21) International Application Number: PCT/US94/05697

(22) International Filing Date: 20 May 1994 (20.05.94)

(71) Applicant *(for all designated States except US)*: UNITED STATES OF AMERICA, represented by THE SECRETARY OF THE ARMY [US/US]; Intellectuel Property Counsel of the Army, Office of The Judge Advocate General, DA, Suite 400, 901 North Stuart Street, Arlington, VA 22203-1837 (US).

(72) Inventors; and

(75) Inventors/Applicants *(for US only)*: REID, Robert, H. [US/US]; 10807 McComas Court, Kensington, MD 20895 (US). SADEGH-NASSERI, Scheherazade [US/US]; 13600 Straw-Bale Lane, Darnestown, MD 20878 (US). WOLFF, Marcia [US/US]; 9850 Hollow Glen Place, Silver Spring, MD 20910 (US). NAUSS, Jeffrey, L. [US/US]; 142 Martha Lane, Fairfield, OH 45014 (US).

(74) Agent: NORRIS, Jerome, J.; Suite 1250, 1401 New York Avenue, N.W., Washington, DC 20005 (US).

(81) Designated States: AT, AU, BB, BG, BR, CA, CH, CZ, DE, DK, ES, FI, GB, HU, JP, KP, KR, LK, LU, MG, MN, MW, NL, NO, NZ, PL, PT, RO, RU, SD, SE, SK, UA, US, European patent (AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE), OAPI patent (BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG).

Published
With international search report.

(54) Title: MODEL FOR TESTING IMMUNOGENICITY OF PEPTIDES

(57) Abstract

Assay methods for determining whether a peptide is likely to be immunogenic are based on a computer modeling of binding to a Class II MHC DR1 receptor. This is confirmed by competitive inhibition binding assays. The peptides are useful for eliciting an immune response for vaccination or the production of antibodies or T-cells.

FOR THE PURPOSES OF INFORMATION ONLY

Codes used to identify States party to the PCT on the front pages of pamphlets publishing international applications under the PCT.

AT	Austria	**GB**	United Kingdom	**MR**	Mauritania
AU	Australia	**GE**	Georgia	**MW**	Malawi
BB	Barbados	**GN**	Guinea	**NE**	Niger
BE	Belgium	**GR**	Greece	**NL**	Netherlands
BF	Burkina Faso	**HU**	Hungary	**NO**	Norway
BG	Bulgaria	**IE**	Ireland	**NZ**	New Zealand
BJ	Benin	**IT**	Italy	**PL**	Poland
BR	Brazil	**JP**	Japan	**PT**	Portugal
BY	Belarus	**KE**	Kenya	**RO**	Romania
CA	Canada	**KG**	Kyrgystan	**RU**	Russian Federation
CF	Central African Republic	**KP**	Democratic People's Republic of Korea	**SD**	Sudan
CG	Congo			**SE**	Sweden
CH	Switzerland	**KR**	Republic of Korea	**SI**	Slovenia
CI	Côte d'Ivoire	**KZ**	Kazakhstan	**SK**	Slovakia
CM	Cameroon	**LI**	Liechtenstein	**SN**	Senegal
CN	China	**LK**	Sri Lanka	**TD**	Chad
CS	Czechoslovakia	**LU**	Luxembourg	**TG**	Togo
CZ	Czech Republic	**LV**	Latvia	**TJ**	Tajikistan
DE	Germany	**MC**	Monaco	**TT**	Trinidad and Tobago
DK	Denmark	**MD**	Republic of Moldova	**UA**	Ukraine
ES	Spain	**MG**	Madagascar	**US**	United States of America
FI	Finland	**ML**	Mali	**UZ**	Uzbekistan
FR	France	**MN**	Mongolia	**VN**	Viet Nam
GA	Gabon				

MODEL FOR TESTING IMMUNOGENICITY OF PEPTIDES

Government Interest

The invention described herein may be manufactured, licensed and used by or for governmental purposes without the payment of any royalties to us thereon.

Cross Reference

This application is a continuation-in-part of U.S. Patent application Serial No. 08/064,559, filed May 21, 1993, and the present application incorporates U.S. Patent Application Serial No. 08/064,559 in its entirety by reference.

Field of the Invention:

This invention relates to a means of predicting potential of a peptide for eliciting immune response.

Background of the Invention:

Among the numerous steps required for an immunological response to occur is the presentation of the antigen by macrophages to the B-cell or T-cell. This presentation is mediated by the Class I and Class II major histocompatibility complex (MHC) molecules on the surface of the cell. The MHC molecules hold antigens in the form of the peptide fragments and together with the receptor molecule on the T-cells, form a macromolecular complex that induces a response in the T-cell. Therefore, a necessary step in an immune response is the binding of the antigen to the MHC.

Recent single crystal X-ray structures of human and murine Class I MHC's have been reported. Analysis of these crystal structures have shown that antigenic peptides lie in the so-called binding cleft for presentation to the T-cell. This cleft is formed by α_1 and α_2 domains and by β-strands from each domain forming the floor. Furthermore, the sequence polymorphism among Class I molecules can result in alterations of the surface of the cleft forming different pockets. Peptide side chains may insert into these pockets. Thus, different pockets may interact with different side chains. This implies the mechanism for the peptide specificity of Class I MHC's. Peptides bound to the Class I MHC's in the crystal structures were found to have both the amino and carboxy termini tightly held by the MHC. There were few interactions near the middle of the cleft. Hence the bound peptide is allowed to bend slightly in the center. The observed binding mode helped to explain the apparent partial specificity of peptide sequence and the allowed variation in peptide length found among peptides isolated from Class I MHC's.

The precise mode of binding of peptides to Class II MHC molecules is less clear. While a single crystal X-ray diffraction structure for the HLA-DR1 MHC has been shown, the coordinates have remained unavailable. However, currently available theoretical and experimental results help form a hypothesis that the binding of a peptide to Class II MHC is similar to that observed with Class I. First, it is noted that the Class II binding cleft is structurally similar to

that of Class I. This was concluded based upon a sequence analysis of 26 Class I and 54 Class II amino acid sequences.

Unlike with Class I molecules, self-peptides isolated from murine I-A^b and I-E^b, from murine I-A^d and from human HLA-DR1 molecules were found to be varied in size (13 to 25 residues long). The peptides isolated from the murine I-A^b and I-E^b molecules had heterogenous carboxy termini while those from I-A^d and HLA-DR1 had ragged termini at both ends. The varying lengths indicate that the amino and carboxy termini of the peptides were not critical for the binding. One or both termini may protrude from the binding site and be available for further processing. The residues critical for binding were proposed to be at the ends of the peptide as opposed to the center.

Summary of the Invention:

It is the purpose of this invention to provide a method for preliminary screening of peptides for ability to elicit an immune response. Structural homology techniques were used to model a receptor (the Class II MHC is exemplified). This model makes it possible to preliminarily screen peptides for antigenic properties. By modifying the peptide to "fit" into the receptor it is possible to identify methods of rendering non-immunogenic peptides immunogenic.

The preliminary screening of peptides for immunogenicity comprises the steps of (1) creating a molecular model of a receptor followed by minimizing the model created, 2) modeling a peptide to be tested and minimizing the model of the peptide, then testing the

fit of the model of the peptide into the model of the receptor to produce a composite minimized receptor/minimized peptide model. Upon finding an acceptable fit, the peptide may then be screened by a binding assay for actual binding to Class II MHC as a further test for immunogenicity.

It has been found that when the model of the peptide can not be fitted into the model of the receptor, the peptide will lack immunogenicity. While not all peptide models which can be made to "fit" into to model of the receptor will be effective as immunogens, the screening methods of the invention may make it possible to avoid undue biological testing of inappropriate peptides. By using the model, it is also possible to alter peptides to accommodate the receptor. Hence, the invention has both predictive and drug design applications.

Brief Description of the Figures:

Fig. 1 shows the HLA-aw68 α_1 and α_2 domains with DR1 α_1 and β_1 domains.

Figs. 2-30 are a printout of the minimized coordinates of the receptor.

Figs. 31 and 32 shows the effects of various peptides inhibiting the binding of labeled hemagglutinin in a competitive binding assay.

Detailed Description of the Invention:

In order to understand and better predict peptide interaction with Class II MHC's and as an aid for synthetic peptide vaccine design, a structural homology model of HLA-DR1 molecule was made

using the Class I HLA-aw68 as a reference molecule. For purposes of this analysis, numerous conserved residues were aligned leading to a proposed three-dimensional model for the Class II structure very similar to that of Class I. This model retained the overall conformation of a Class I MHC and agreed with a considerable amount of the published data. Furthermore, peptides shown to bind to DR1 were docked in the binding cleft of the model and analyzed. The results agree with the experimental binding data presented here. Hence, it is shown that the structural homology model reported here is useful for screening Class II MHC functionality.

It had been hypothesized that few peptide residues may be required for binding to DR1. By substituting residues into the influenza hemagglutinin 307-319 T-cell epitope (HA) it had been determined that a single tyrosine at 308 was required for binding. A synthetic peptide with the tyrosine at position 308 and a lysine at 315 was found to bind DR1 as well as the native peptide. Hence, it was concluded that few peptide residues determine the high affinity binding to DR1.

The peptides produced according to the present invention may be used alone or chemically bound to another peptide and/or carrier in order to elicit an immune response. An immune response is elicited by administering a peptide to an animal in an effective dose and by an effective route of administration. Typically the peptide will be administered with an immunologically acceptable carrier. The routes of administration, dosages, times between multiple administrations will be based on the particular peptide and are standard operations of those skilled in the art.

Of particular interest are peptides from pathogenic microorganisms and neoplasms. In such an example, a vaccine may be formed with the peptide and any known immunological carrier and may be administered prophylactically or therapeutically. The immune response may be elicited for a number of reasons other than for prophylaxis or therapy such as increasing antibody production for the harvesting of antibodies, or increasing specific B-cell or T-cell concentration for the production of hybridomas or cellular therapy.

The choice of host animals is limited only to those capable of an immune response. Preferred hosts are mammals, more preferred are humans.

The vaccine may contain plural peptides with each peptide corresponding to the same or different antigens. The peptides may be used unbound or they may be chemically bound to another peptide or an unrelated protein or other molecule. A preferred vaccine preparation contains a plurality of peptides chemically bound to a larger more immunogenic peptide.

The peptide may be adsorbed, bound or encapsulated in a biodegradeable microsphere, microcapsule, larger carrier or a combination of these. The carrier may have a slow or controlled release property thereby releasing the peptide under appropriate conditions and times for enhanced immunization. This is particularly important when administering the peptide orally where stomach acid can degrade the peptide.

Another embodiment of the present invention is to modify the amino acid sequence of a peptide to enhance its immunogenicity. This is done by modifying the natural peptide sequence to bind to

the Class II MHC receptor DR1 with superior binding affinity for a Class II MHC receptor DR1 than the natural peptide sequence. This modified peptide is considered a synthetic peptide. Alternatively, the sequence may be modified to have a greater inhibition of HA (306-318) binding to a Class II MHC receptor DR1.

Many amino acid changes are acceptable in the formation of a synthetic peptide. The changes may be for similar types of amino acids such as leucine for isoleucine or they may be for diverse types such as tyrosine for lysine.

Materials and Methods:

The structural homology model for the DR1 Class II MHC was constructed using the QUANTA molecular modeling package (vision 3.2, Molecular Simulations, Inc., Burlington, MA) with the CHARMM and Protein Design modules. After alignment of the sequences as described below, gaps and loops were energy minimized using 100 steps of steepest descents minimization followed by 100 steps of adopted basis set Newton-Rapheson (ABNR) minimization. Large gaps were closed using a fragment database from a selected set of high-resolution crystal structures. The resulting structure was minimized in vacuo using 1000 steps of steepest descents followed by an additional 1000 steps of ABNR minimization. A distance related electrostatic function was used in all calculations with a dielectric constant of 1.0. Non-bound parameter lists were updated every 20 steps with a cutoff distance of 15.0Å. Non-bonded calculations were performed using a shifted potential function between 11.0Å and 14.0Å. An extended atom set was used with only

polar hydrogen atoms specifically placed. There were no explicit hydrogen bond energy calculations performed.

All peptides were initially modeled using QUANTA in an extended chain conformation and subjected to 500 steps of ABNR minimization. The resulting structures remained essentially in extended chain conformations. Individual peptides were manually docked in several different orientations into the binding cleft region of the minimized DR1 structure. The resulting bimolecular complex was subjected to 5000 steps of steepest descents minimization with non-bonded interactions updated every five steps. After minimization, bound peptides remained essentially in extended chain conformations. The lowest energy complexes for each peptide were selected for further analysis.

The selected peptide and DR1 complexes and the minimized DR1 model were subjected to the following molecular dynamics regimen: 300 steps of heating to 300°K, 600 steps of equilibration at 300°K, and 1100 steps of production dynamics. During this simulation, the DR1 Cα atoms were constrained in their starting positions. All non-bonded interaction parameters were as stated for the minimization procedure. The lowest energy structure during the course of the production dynamics was selected and subjected to the 5000 step minimization procedure described previously with the Cα restraints removed. The resulting structures were used for the binding energy calculations and for hydrogen bonding analysis.

Hydrogen bonds were determined using the QUANTA default parameters. Maximum allowed distances were 2.5Å between a hydrogen and the acceptor atom and 3.3Å between the donor and acceptor atoms.

The minimum angle allowed between any set of atoms forming a hydrogen bond was 90°.

Competitive Inhibition Binding Assay:

HA peptide (the influenza hemagglutinin 307-319 T-cell epitope) was labeled with ^{125}I. The labeled HA peptides were then allowed to interact with purified DR1 molecules during incubation to allow formation of peptide/DR1 complexes. After incubation, the peptide/DR1 composition was exposed to a native gel for chromatographic separation or passed through a spun column to separate labeled peptide/DR1 complex and free labelled peptide. When unlabeled peptides were added before incubation of labeled HA peptides and DR1, and if the unlabelled peptides had capacity for binding to DR1 simultaneous with ^{125}I-HA, there was a resultant decrease in radioactive signal associated with the DR1. The extent of this decrease directly related to the binding capacity of the unlabeled unknown peptide.

Structural Homology Model for the DR1 Molecule:

The structural homology model was created, the reference molecule being the crystal structure of HLA-aw68. The HLA-aw68 coordinates and subsequent sequence were obtained from the entry 2HLA in the Brookhaven Protein Data Bank released January 15, 1991, which is incorporated herein by reference. The sequence for the DR1 molecule was for the α_1 domain was reported by Klein and for the β_1 domain, the study reported by Todd et al. (Nature 329, 599 (1987)).

The sequence alignment is based on Brown et al. (Nature 332, 845 (1988)). The complete alignment and numbering scheme for both

are seen in Figure 1. The Class II, β_1 and Class I α_2 domains regions were conserved with some variations at the ends where the two MHC's have different loop regions. The fourth B-strand in the α_1 domain of HLA-aw68 (residues 30-38) is disrupted in the DR1 model. Only three residues are in a β-sheet conformation, probably due to the inserted glycine at position 28 before the strand and the large deletion in the loop region immediately after the strand. The two alpha-helical regions are clearly maintained. Both helices have been observed to be discontinuous in the Class I molecules and are similar in the DR1 model. The α_1 domain helix is long and curves from residues 49α to 76α without significant disruption. It is essentially a single continuous helix. However, the α_2 helical region is broken into two separate helices as with the Class I molecules. A short helix (52-63) is separated from a longer helix (68-94) by a deformed region without secondary structure. This deformation is more pronounced in the DR1 model as opposed to the Class I molecules due to an insertion.

Influenza Hemagglutinin Peptide with DR1:

The amino acid residues 307-319 of influenza hemagglutinin (Pro-Lys- Tyr-Val-Lys-Gln-Asn-Thr-Leu-Lys-Leu-Ala-Thr) make up a well-documented linear T-cell epitope which has been shown to be HLA-DR1 restricted. With the demonstration that the influenza hemagglutinin epitope (referred to as the HA peptide) binds DR1, it was chosen to be modeled into the binding cleft.

The peptide was initially inserted into the cleft so that Leu 11 HA was in the vicinity of the hydrophobic pocket. This allowed Asn 7 to be near the middle charged and polar groups of the cleft.

The remaining residue of the motif (Lys 2) was near the vicinity of the remaining charged and polar residues at the end of the cleft. The only adjustment to the starting conformation was a slight rearrangement of the terminal peptide proline and Tyr 3 to alleviate obvious bad contacts.

After the energy minimization of the bimolecular complex, the total energy was reduced to 483 kcal/mol. This reduction in energy was accomplished by alleviation of several bad contacts and also be formation of several hydrogen bonds. The sticking feature of this mode is lack of hydrogen bonds in the carboxy terminal half of the peptide. Only one hydrogen bond is identified between the backbone carbonyl group of Leu 9 and the side chain of the β_1 Asn 77. In contrast, the amino terminal half has eleven identified interactions. Four of these interaction involve the peptide backbone residues Tyr 3, Val 4, and Gln 6. The remainder involve the side chains of Lys 2, Tyr 3, Lys 5 and Gln 6. Interestingly, Lys 5 is involved in more interactions (three) than Lys 2 (only 2). No interactions were observed as anticipated with Asn 7. Instead, it was the glutamine at position 6 donating a hydrogen bond to the α_1 Asn 62. No interactions were observed for the amino and carboxy termini.

HA-YK Peptide with DR1:

The binding of the HA-YK peptide (Ala-Ala-Tyr-Ala-Ala-Ala-Ala-Ala-Ala-Lys-Ala-Ala) to the DR1 model was tested. In aligning the peptide in the cleft, it was deemed logical to insert the tyrosine residue into the hydrophobic region of the binding cleft. The lysine would then be in position to interact with the

hydrophilic groups in the other half of the cleft. The resulting peptide orientation is the opposite that used for the HA and the CS3 (defined below) peptides. With the peptide oriented as described, the final docking position for the peptide was unclear. The hydrophobic pocket is quite large, and, at least in this model, could accommodate the peptide tyrosine in a number of positions by sliding the peptide lengthwise through the cleft. However, repositioning the peptide also repositions the lysine. There were primarily two positions for the lysine: one with the lysine inside the cleft and the second with it outside. Of the two positions, the former was the lower in energy by 46 kcal/mol and had the greater number of interactions with the protein (11 vs. 7). Thus, the preferred orientation of the peptide appears to be with the lysine inside the binding cleft region.

CS3 subunit Pilin Peptide with DR1:

The suspected T-cell epitope for CS3 pilus subunit 63-78 (Ser-Lys-Asn-Gly-Thr-Val-Thr-Trp-Ala-His-Glu-Thr-Asn-Asn-Ser-Ala) was modeled with the DR1 molecule. The peptide was inserted with lysine inside the cleft in the hydrophilic region. This placed the Thr 5 in the center of the binding cleft and the tryptophane (residue 8) near the hydrophobic region. The resulting minimized model had ten interactions between the peptide and the protein, three interactions with the peptide backbone and five with the peptide side chains. The remaining two were with the amino terminal of the peptide. All of the interactions were in either the first three residues, His 10 or Glu 11 in the peptide. No interactions

were observed in the center of the cleft or residues four through nine.

CFA/1 with DR1:

A peptide identified as CFA/1 (colonization factor antigen) (Val-Gly-Lys-Asn-Ile-Thr-Val-Thr-Ala-Ser-Val-Asp-Pro) was prepared and an attempt was made to "fit" the molecule into the cleft of the DR1. The lysine at position 3 prevented insertion of the peptide.

Results:

The peptides chosen to dock in the DR1 model are shown in Table 1. The peptides were docked manually in several orientations into the DR1 model. The peptides were then tested in biological binding assays with the following results:

Table I

Peptide	Molecular Model predicted binding	Binding in the bioassay
HA (influenza hemagglutinin)	Yes	Yes
HA-YK (synthetic peptide)	Yes	Yes
CS3 Pilin subunit	Yes	Yes
CFA/1	No	No

Quantitative measurement of the inhibition of CS3 63-78 and HA 306-318 as compared to controls is shown in Fig. 31.

The binding energy was calculated as the difference between the final DR1 and peptide complex and the sum of the energies for the minimized DR and peptide models individually. The data is shown in Table II.

Table II.

Peptide	Protein	Residues	Sequence	Binding Energy (kcal/mol)
HA	Influenza hemagglutinin	306-318	PKYVKQNTLKLAT	-283
HA-YK	synthetic peptide		AAYAAAAAAKAA	-216
CS3	CS3 pilin subunit	63-78	SKNGTVTWAHETNNSA	-245

CS6α and CS6ß with DR1

Colonization factor antigen IV (CFA/IV is an antigen on the surface of many enterotoxigenic *E. coli* one component of which is CS6. CS6 has two major subunits and a number of minor subunits. Several peptides from CS6 have been sequenced and assayed for potential inhibition of radiolabeled HA (306-318)/DR1 complex as a measure of immunogenicity. The sequences of the subunits are shown in Table III.

Table III.

Peptide	Amino Acid Residues	Sequence
CS6α6	63-75	DEYGLGRLVNTAD
CS6α7	80-92	IIYQIVDEKGKKK
CS6α8	111-123	LNYTSGEKKISPG
CS6ß1	3-15	WQYKSLDVNVNIE
CS6ß2	42-54	QLYTVEMTIPAGV
CS6ß3	112-124	TSYTFSAIYTGGE
CS6ß4	123-135	GEYPNSGYSSGTY
CS6ß5	133-145	GTYAGHLTVSFYS

These peptides were assayed for inhibition of radioactively labeled HA(306-318)/DR1. The results are demonstrated in Fig. 32.

The foregoing description of the specific embodiments reveal the general nature of the invention so that others can, by applying current knowledge, readily modify and/or adapt for various applications such specific embodiments without departing from the generic concept, and, therefore, such adaptations and modifications should and are intended to be comprehended within the meaning and range of equivalents of the disclosed embodiments. It is to be understood that the phraseology or terminology employed herein is for the purpose of description and not of limitation.

All references mentioned in this application are incorporated by reference.

We Claim:

1. A method of preliminarily screening peptides for immunogenicity comprising the steps of:

1) creating a molecular model of receptor DR1 Class II MHC and minimizing the model of the DR1;

2) modeling a peptide to be tested and minimizing the model of the peptide; and

3) testing fit of model obtained in step 2 into the model obtained in step 1 to produce a composite receptor/peptide model.

2. A computerized model comprising a model of the DR1 molecule having fitted in a cleft therein a model of a peptide.

3. A method of claim 1 wherein, additionally, the receptor/peptide model is subjected to computer-simulated heating.

4. A method of claim 1 further comprising, assaying the peptide by competitive inhibition binding to a Class II MHC receptor DR1.

5. A minimized peptide capable of binding to a Class II MHC receptor DR1 and inhibiting the binding of HA (306-318).

6. A synthetic peptide, wherein the amino acid sequence of the minimized peptide according to claim 5 has been modified to have a superior binding affinity for a Class II MHC receptor DR1 to form at least a portion of the synthetic peptide.

7. A synthetic peptide, wherein the amino acid sequence of the minimized peptide according to claim 5, has been modified to have greater inhibition of HA (306-318) binding to a Class II MHC receptor DR1 to form at least a portion of the synthetic peptide.

8. A synthetic peptide according to claim 6, wherein an amino acid has been modified from a charged amino acid to an uncharged amino acid.

9. A synthetic peptide according to claim 7, wherein an amino acid has been modified from a charged amino acid to an uncharged amino acid.

10. A synthetic peptide according to claim 8, wherein said uncharged amino acid is alanine.

11. A synthetic peptide according to claim 9, wherein said uncharged amino acid is alanine.

12. A minimized peptide according to claim 5, wherein the sequence is selected from the group consisting of PKYVKQNTLKLAT, AAYAAAAAAKAA and SKNGTVTWAHETNNSA.

13. A minimized peptide according to claim 5, wherein the sequence is contained in a CFA.

14. A minimized peptide according to claim 13, wherein the sequence is selected from the group consisting of DEYGLGRLVNTAD, IIYQIVDEKGKKK, LNYTSGEKKISPG, WQYKSLDVNVNIE, QLYTVEMTIPAGV, TSYTFSAIYTGGE, GEYPNSGYSSGTY and GTYAGHLTVSFYS.

15. A vaccine comprising:
a minimized peptide according to claim 5; and
an immunologically acceptable carrier.

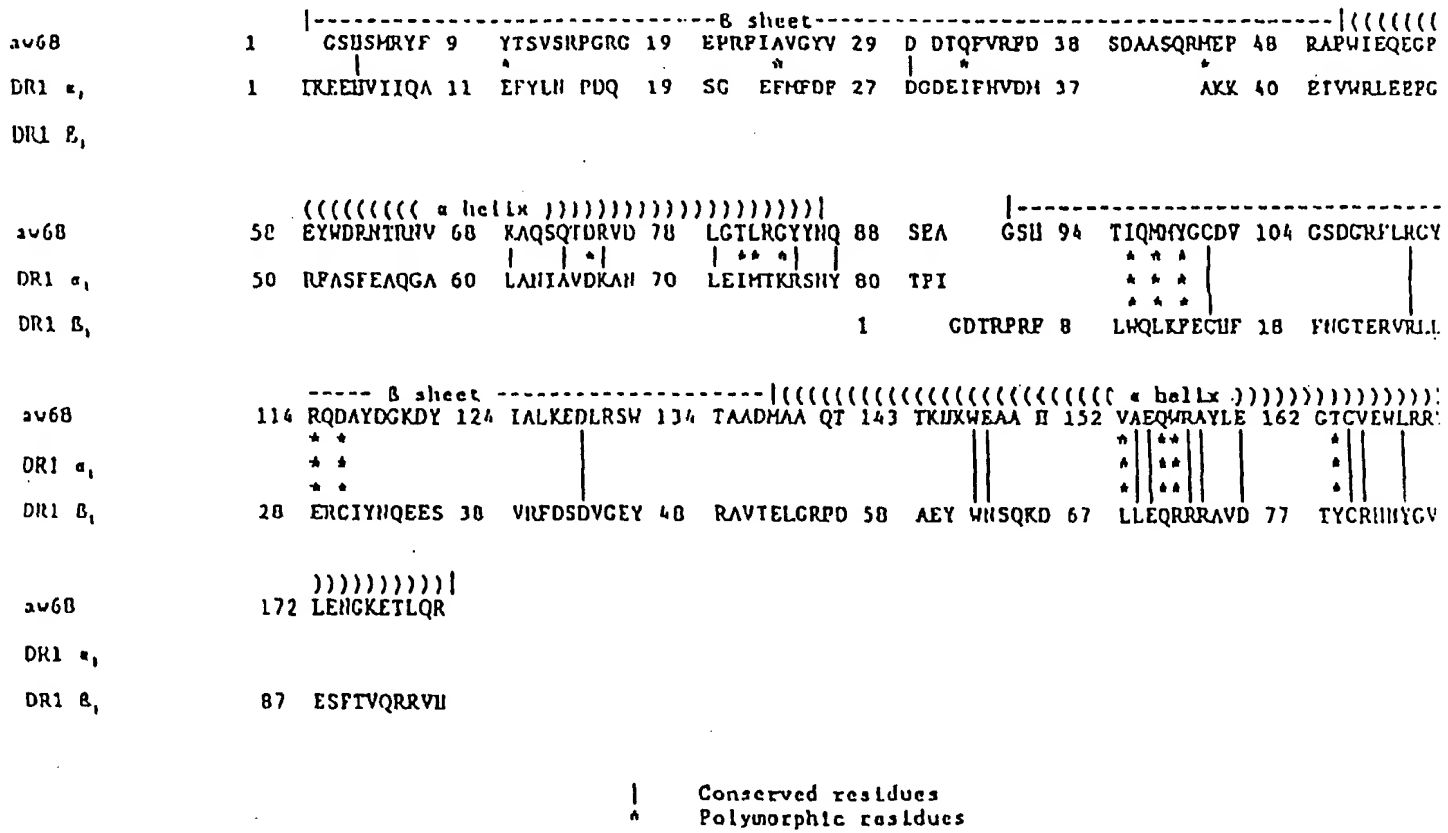
16. A vaccine comprising:
a synthetic peptide according to claim 6; and
an immunologically acceptable carrier.

17. A vaccine comprising:
a synthetic peptide according to claim 7; and
an immunologically acceptable carrier.

18. A method of eliciting an immune response in an animal comprising administering said animal with the vaccine according to claim 15.

19. A method of eliciting an immune response in an animal comprising administering said animal with the vaccine according to claim 16.

20. A method of eliciting an immune response in an animal comprising administering said animal with the vaccine according to claim 17.



| Conserved residues
* Polymorphic residues

FIG. 1

```
* MINIMIZED COORDINATES FROM CHARMM
*  DATE:     2/25/93     14:58:48      CREATED BY USER: nbus*
*
 1639
    1     1 ILE  N     -53.41835 -52.07964  96.86949 A1   1      0.00000
    2     1 ILE  HT1   -54.06550 -53.37379  96.22549 A1   1      0.00000
    3     1 ILE  HT2   -52.48505 -53.33354  96.89426 A1   1      0.00000
    4     1 ILE  HT3   -53.81151 -52.85195  97.84341 A1   1      0.00000
    5     1 ILE  CA    -53.29159 -51.45945  96.52548 A1   1      0.00000
    6     1 ILE  CB    -54.51076 -51.09296  95.64551 A1   1      0.00000
    7     1 ILE  CG2   -55.84867 -51.39510  96.33544 A1   1      0.00000
    8     1 ILE  CG1   -54.43380 -49.65164  95.12978 A1   1      0.00000
    9     1 ILE  CD    -55.55018 -49.30658  94.14124 A1   1      0.00000
   10     1 ILE  C     -53.31306 -50.79352  97.88119 A1   1      0.00000
   11     1 ILE  O     -53.76732 -51.45486  98.80000 A1   1      0.00000
   12     2 LYS  N     -52.70566 -49.57271  97.98462 A1   2      0.00000
   13     2 LYS  H     -52.43149 -49.07042  97.19065 A1   2      0.00000
   14     2 LYS  CA    -52.72856 -48.82990  99.24363 A1   2      0.00000
   15     2 LYS  CB    -51.40674 -49.22996 100.05168 A1   2      0.00000
   16     2 LYS  CG    -51.65942 -50.46422 100.94226 A1   2      0.00000
   17     2 LYS  CD    -50.39491 -50.76541 101.74483 A1   2      0.00000
   18     2 LYS  CE    -50.65567 -51.67024 102.94896 A1   2      0.00000
   19     2 LYS  NZ    -49.48784 -51.62033 103.84066 A1   2      0.00000
   20     2 LYS  HZ1   -49.68891 -52.15413 104.71032 A1   2      0.00000
   21     2 LYS  HZ2   -48.66152 -52.03086 103.36182 A1   2      0.00000
   22     2 LYS  HZ3   -49.20787 -50.62863 104.08530 A1   2      0.00000
   23     2 LYS  C     -52.58080 -47.37619  98.85749 A1   2      0.00000
   24     2 LYS  O     -52.16561 -47.08993  97.74074 A1   2      0.00000
   25     3 GLU  N     -52.93375 -46.48610  99.78817 A1   3      0.00000
   26     3 GLU  H     -53.25920 -46.74733 100.69754 A1   3      0.00000
   27     3 GLU  CA    -52.88416 -45.05669  99.49342 A1   3      0.00000
   28     3 GLU  CB    -54.17633 -44.67728  98.75869 A1   3      0.00000
   29     3 GLU  CG    -54.16941 -43.30721  98.07127 A1   3      0.00000
   30     3 GLU  CD    -55.38365 -43.14982  97.16830 A1   3      0.00000
   31     3 GLU  OE1   -55.40070 -42.20412  96.38367 A1   3      0.00000
   32     3 GLU  OE2   -56.30088 -43.96983  97.23742 A1   3      0.00000
   33     3 GLU  C     -52.73723 -44.30588 100.80334 A1   3      0.00000
   34     3 GLU  O     -53.13310 -44.80289 101.85375 A1   3      0.00000
   35     4 GLU  N     -52.10513 -43.13147 100.72198 A1   4      0.00000
   36     4 GLU  H     -51.89913 -42.70887  99.83885 A1   4      0.00000
   37     4 GLU  CA    -51.71490 -42.41569 101.93532 A1   4      0.00000
   38     4 GLU  CB    -50.23606 -42.65775 102.23912 A1   4      0.00000
   39     4 GLU  CG    -49.88908 -44.07273 102.69972 A1   4      0.00000
   40     4 GLU  CD    -48.39447 -44.20822 102.86978 A1   4      0.00000
   41     4 GLU  OE1   -47.71593 -43.20739 103.12446 A1   4      0.00000
   42     4 GLU  OE2   -47.87485 -45.31826 102.72475 A1   4      0.00000
   43     4 GLU  C     -51.86859 -40.92476 101.75610 A1   4      0.00000
   44     4 GLU  O     -51.85445 -40.40438 100.64776 A1   4      0.00000
   45     5 HIS  N     -51.98758 -40.25490 102.89941 A1   5      0.00000
   46     5 HIS  H     -51.95529 -40.74179 103.77267 A1   5      0.00000
   47     5 HIS  CA    -52.02510 -38.79739 102.88794 A1   5      0.00000
   48     5 HIS  CB    -52.95268 -38.30654 104.00423 A1   5      0.00000
   49     5 HIS  CG    -54.39292 -38.58657 103.64511 A1   5      0.00000
   50     5 HIS  ND1   -55.01336 -38.04007 102.58831 A1   5      0.00000
   51     5 HIS  HD1   -54.63216 -37.40030 101.93314 A1   5      0.00000
   52     5 HIS  CD2   -55.29163 -39.42491 104.31043 A1   5      0.00000
   53     5 HIS  NE2   -56.46563 -39.37373 103.63249 A1   5      0.00000
   54     5 HIS  CE1   -56.29489 -38.51954 102.57197 A1   5      0.00000
   55     5 HIS  C     -50.64149 -38.20241 103.06558 A1   5      0.00000
   56     5 HIS  O     -49.75908 -38.78174 103.68940 A1   5      0.00000
   57     6 VAL  N     -50.46014 -37.02655 102.46317 A1   6      0.00000
   58     6 VAL  H     -51.22869 -36.59864 101.97707 A1   6      0.00000
   59     6 VAL  CA    -49.12695 -36.41474 102.46428 A1   6      0.00000
   60     6 VAL  CB    -48.60121 -36.33669 101.01420 A1   6      0.00000
```

FIG. 2

61	6	VAL	CG1	47.07672	-36.30119	101.00126	A1	6	0.00000
62	6	VAL	CG2	49.10544	-37.46647	100.11057	A1	6	0.00000
63	6	VAL	C	-49.19435	-35.00190	103.02675	A1	6	0.00000
64	6	VAL	O	-50.21018	-34.34041	102.87457	A1	6	0.00000
65	7	ILE	N	-48.11527	-34.52120	103.65431	A1	7	0.00000
66	7	ILE	H	-47.35972	-35.13148	103.91409	A1	7	0.00000
67	7	ILE	CA	-48.09506	-33.08697	103.98819	A1	7	0.00000
68	7	ILE	CB	-48.69197	-32.86813	105.39701	A1	7	0.00000
69	7	ILE	CG2	-47.96322	-33.71317	106.43001	A1	7	0.00000
70	7	ILE	CG1	-48.76316	-31.39586	105.81727	A1	7	0.00000
71	7	ILE	CD	-49.28846	-31.20489	107.23523	A1	7	0.00000
72	7	ILE	C	-46.69381	-32.50114	103.87753	A1	7	0.00000
73	7	ILE	O	-45.72315	-33.10109	104.32366	A1	8	0.00000
74	8	ILE	N	-46.61414	-31.32789	103.23109	A1	8	0.00000
75	8	ILE	H	-47.43598	-30.79777	103.00074	A1	8	0.00000
76	8	ILE	CA	-45.31176	-30.85113	102.75879	A1	8	0.00000
77	8	ILE	CB	-45.18096	-31.21426	101.24826	A1	8	0.00000
78	8	ILE	CG2	-46.47692	-30.98133	100.47371	A1	8	0.00000
79	8	ILE	CG1	-44.01581	-30.53590	100.51961	A1	8	0.00000
80	8	ILE	CD	-42.65515	-30.85297	101.12422	A1	8	0.00000
81	8	ILE	C	-45.00402	-29.37643	103.03239	A1	8	0.00000
82	8	ILE	O	-45.69216	-28.43922	102.63903	A1	8	0.00000
83	9	GLN	N	-43.86371	-29.19466	103.70229	A1	9	0.00000
84	9	GLN	H	-43.33777	-29.97409	104.05676	A1	9	0.00000
85	9	GLN	CA	-43.27910	-27.85712	103.71549	A1	9	0.00000
86	9	GLN	CB	-42.97213	-27.43231	105.14730	A1	9	0.00000
87	9	GLN	CG	-44.24353	-27.13894	105.94550	A1	9	0.00000
88	9	GLN	CD	-43.92932	-26.69043	107.36359	A1	9	0.00000
89	9	GLN	OE1	-44.59992	-27.05224	108.31811	A1	9	0.00000
90	9	GLN	NE2	-42.89278	-25.86874	107.50418	A1	9	0.00000
91	9	GLN	HE21	-42.31986	-25.58069	106.73881	A1	9	0.00000
92	9	GLN	HE22	-42.66204	-25.53260	108.41526	A1	9	0.00000
93	9	GLN	C	-42.00840	-27.79728	102.89330	A1	9	0.00000
94	9	GLN	O	-41.07030	-28.56703	103.06902	A1	10	0.00000
95	10	ALA	N	-42.01720	-26.84230	101.96835	A1	10	0.00000
96	10	ALA	H	-42.80016	-26.24022	101.81084	A1	10	0.00000
97	10	ALA	CA	-40.83464	-26.60034	101.15833	A1	10	0.00000
98	10	ALA	CB	-41.09424	-26.95993	99.69281	A1	10	0.00000
99	10	ALA	C	-40.41733	-25.14834	101.25674	A1	10	0.00000
100	10	ALA	O	-41.21138	-24.24680	101.50542	A1	11	0.00000
101	11	GLU	N	-39.11637	-24.95043	101.08226	A1	11	0.00000
102	11	GLU	H	-38.51800	-25.72332	100.86462	A1	11	0.00000
103	11	GLU	CA	-38.56697	-23.61077	101.26935	A1	11	0.00000
104	11	GLU	CB	-37.61570	-23.62729	102.46404	A1	11	0.00000
105	11	GLU	CG	-38.29740	-24.15021	103.73032	A1	11	0.00000
106	11	GLU	CD	-37.31724	-24.35236	104.86668	A1	11	0.00000
107	11	GLU	OE1	-37.72498	-24.91514	105.87939	A1	11	0.00000
108	11	GLU	OE2	-36.15746	-23.95826	104.74301	A1	11	0.00000
109	11	GLU	C	-37.79619	-23.17941	100.04756	A1	11	0.00000
110	11	GLU	O	-37.17390	-23.99314	99.37097	A1	12	0.00000
111	12	PHE	N	-37.86688	-21.87280	99.78525	A1	12	0.00000
112	12	PHE	H	-38.38856	-21.25141	100.37827	A1	12	0.00000
113	12	PHE	CA	-37.20863	-21.33691	98.59813	A1	12	0.00000
114	12	PHE	CB	-38.26225	-21.06791	97.51950	A1	12	0.00000
115	12	PHE	CG	-37.93682	-21.86124	96.27668	A1	12	0.00000
116	12	PHE	CD1	-38.35291	-23.20899	96.17465	A1	12	0.00000
117	12	PHE	CD2	-37.21678	-21.25353	95.22261	A1	12	0.00000
118	12	PHE	CE1	-38.04712	-23.95258	95.01356	A1	12	0.00000
119	12	PHE	CE2	-36.91098	-21.99741	94.06122	A1	12	0.00000
120	12	PHE	CZ	-37.32685	-23.34453	93.96022	A1	12	0.00000
121	12	PHE	C	-36.45949	-20.05659	98.90209	A1	12	0.00000
122	12	PHE	O	-37.00216	-18.95808	98.93077	A1	13	0.00000
123	13	TYR	N	-35.16677	-20.22034	99.15293	A1	13	0.00000
124	13	TYR	H	-34.71888	-21.10896	99.03348	A1		

FIG. 3

./DR1_MD2.CRD Sat Feb 25 14:58:48 1995 3

125	13	TYR	CA	4.44650	-19.02891	99.57908	A1	13	0.00000
126	13	TYR	CB	-33.74164	-19.31637	100.90471	A1	13	0.00000
127	13	TYR	CG	-33.63229	-18.04844	101.71489	A1	13	0.00000
128	13	TYR	CD1	-34.79192	-17.52707	102.32828	A1	13	0.00000
129	13	TYR	CE1	-34.69736	-16.35710	103.10470	A1	13	0.00000
130	13	TYR	CD2	-32.38328	-17.40687	101.86606	A1	13	0.00000
131	13	TYR	CE2	-32.29405	-16.23332	102.64552	A1	13	0.00000
132	13	TYR	CZ	-33.45188	-15.71594	103.26657	A1	13	0.00000
133	13	TYR	OH	-33.37191	-14.58930	104.06109	A1	13	0.00000
134	13	TYR	HH	-33.47343	-14.89238	104.98360	A1	13	0.00000
135	13	TYR	C	-33.46702	-18.52544	98.54525	A1	13	0.00000
136	13	TYR	O	-32.59456	-19.23915	98.06786	A1	13	0.00000
137	14	LEU	N	-33.65240	-17.25550	98.19697	A1	14	0.00000
138	14	LEU	H	-34.33538	-16.68306	98.64807	A1	14	0.00000
139	14	LEU	CA	-32.81168	-16.70428	97.14258	A1	14	0.00000
140	14	LEU	CB	-33.70274	-16.21044	96.00105	A1	14	0.00000
141	14	LEU	CG	-33.98219	-17.29674	94.96260	A1	14	0.00000
142	14	LEU	CD1	-35.16863	-16.92524	94.07539	A1	14	0.00000
143	14	LEU	CD2	-32.72461	-17.54798	94.13078	A1	14	0.00000
144	14	LEU	C	-31.93377	-15.56813	97.60481	A1	14	0.00000
145	14	LEU	O	-32.31049	-14.71998	98.40126	A1	14	0.00000
146	15	ASN	N	-30.73908	-15.58168	97.02166	A1	15	0.00000
147	15	ASN	H	-30.47955	-16.38705	96.48149	A1	15	0.00000
148	15	ASN	CA	-29.88530	-14.39297	97.02352	A1	15	0.00000
149	15	ASN	CB	-28.47094	-14.93729	97.29287	A1	15	0.00000
150	15	ASN	CG	-27.86774	-14.18957	98.46652	A1	15	0.00000
151	15	ASN	OD1	-28.47231	-13.98878	99.50693	A1	15	0.00000
152	15	ASN	ND2	-26.63329	-13.74712	98.26721	A1	15	0.00000
153	15	ASN	HD21	-26.12722	-13.93409	97.42633	A1	15	0.00000
154	15	ASN	HD22	-26.21377	-13.18778	98.98020	A1	15	0.00000
155	15	ASN	C	-30.09328	-13.70870	95.65633	A1	15	0.00000
156	15	ASN	O	-30.96066	-14.17939	94.92357	A1	15	0.00000
157	16	PRO	N	-29.35358	-12.64312	95.25454	A1	16	0.00000
158	16	PRO	CD	-29.47390	-12.14147	93.88390	A1	16	0.00000
159	16	PRO	CA	-28.34388	-11.89943	96.02164	A1	16	0.00000
160	16	PRO	CB	-27.47317	-11.32145	94.90180	A1	16	0.00000
161	16	PRO	CG	-28.40713	-11.06430	93.72211	A1	16	0.00000
162	16	PRO	C	-28.87201	-10.84560	96.98393	A1	16	0.00000
163	16	PRO	O	-28.49727	-10.81095	98.14625	A1	16	0.00000
164	17	ASP	N	-29.73099	-9.96981	96.45979	A1	17	0.00000
165	17	ASP	H	-30.06531	-10.06794	95.52595	A1	17	0.00000
166	17	ASP	CA	-30.07647	-8.75629	97.18869	A1	17	0.00000
167	17	ASP	CB	-30.80318	-7.83976	96.20071	A1	17	0.00000
168	17	ASP	CG	-30.22601	-6.44601	96.27578	A1	17	0.00000
169	17	ASP	OD1	-29.42577	-6.10216	95.40955	A1	17	0.00000
170	17	ASP	OD2	-30.58500	-5.71147	97.19272	A1	17	0.00000
171	17	ASP	C	-30.91226	-8.96778	98.44177	A1	17	0.00000
172	17	ASP	O	-30.52677	-8.65960	99.56331	A1	17	0.00000
173	18	GLN	N	-32.11780	-9.49744	98.20428	A1	18	0.00000
174	18	GLN	H	-32.36542	-9.81984	97.29256	A1	18	0.00000
175	18	GLN	CA	-33.10696	-9.57864	99.27949	A1	18	0.00000
176	18	GLN	CB	-34.05728	-8.37464	99.14180	A1	18	0.00000
177	18	GLN	CG	-33.36307	-7.07517	99.58476	A1	18	0.00000
178	18	GLN	CD	-33.97880	-5.85158	98.94046	A1	18	0.00000
179	18	GLN	OE1	-35.13776	-5.50918	99.12725	A1	18	0.00000
180	18	GLN	NE2	-33.14378	-5.16835	98.16624	A1	18	0.00000
181	18	GLN	HE21	-32.19859	-5.47544	97.99847	A1	18	0.00000
182	18	GLN	HE22	-33.43475	-4.32502	97.72302	A1	18	0.00000
183	18	GLN	C	-33.83924	-10.91598	99.26964	A1	18	0.00000
184	18	GLN	O	-33.74750	-11.68763	98.32391	A1	18	0.00000
185	19	SER	N	-34.51482	-11.16924	100.39831	A1	19	0.00000
186	19	SER	H	-34.63228	-10.43017	101.06649	A1	19	0.00000
187	19	SER	CA	-34.94474	-12.50616	100.83625	A1	19	0.00000
188	19	SER	CB	-35.43672	-12.36114	102.28173	A1	19	0.00000

FIG. 4

189	19	SER	OG	34.37064	-11.87727	103.10841	A1	19	0.00000
190	19	SER	HG	33.63984	-12.63499	103.40254	A1	19	0.00000
191	19	SER	C	-35.97640	-13.29776	100.02197	A1	19	0.00000
192	19	SER	O	-36.49518	-12.86400	99.00144	A1	19	0.00000
193	20	GLY	N	-36.24917	-14.51787	100.53004	A1	20	0.00000
194	20	GLY	H	-35.87834	-14.79673	101.41380	A1	20	0.00000
195	20	GLY	CA	-37.08223	-15.47533	99.79192	A1	20	0.00000
196	20	GLY	C	-38.39897	-15.89747	100.44590	A1	20	0.00000
197	20	GLY	O	-39.10838	-15.10421	101.05171	A1	20	0.00000
198	21	GLU	N	-38.72023	-17.18722	100.25477	A1	21	0.00000
199	21	GLU	H	-38.03254	-17.84573	99.94375	A1	21	0.00000
200	21	GLU	CA	-40.11538	-17.64629	100.27114	A1	21	0.00000
201	21	GLU	CB	-40.54163	-17.64420	98.79559	A1	21	0.00000
202	21	GLU	CG	-42.00974	-17.90322	98.44054	A1	21	0.00000
203	21	GLU	CD	-42.16555	-17.98331	96.93169	A1	21	0.00000
204	21	GLU	OE1	-43.22010	-17.59671	96.43390	A1	21	0.00000
205	21	GLU	OE2	-41.23758	-18.43207	96.25678	A1	21	0.00000
206	21	GLU	C	-40.28326	-19.04137	100.89226	A1	21	0.00000
207	21	GLU	O	-39.32286	-19.78361	101.07437	A1	21	0.00000
208	22	PHE	N	-41.54286	-19.38051	101.22645	A1	22	0.00000
209	22	PHE	H	-42.30204	-18.76344	101.01655	A1	22	0.00000
210	22	PHE	CA	-41.84777	-20.63223	101.93252	A1	22	0.00000
211	22	PHE	CB	-41.76716	-20.31207	103.43794	A1	22	0.00000
212	22	PHE	CG	-41.45246	-21.48591	104.34752	A1	22	0.00000
213	22	PHE	CD1	-40.59481	-21.25886	105.44915	A1	22	0.00000
214	22	PHE	CD2	-42.01384	-22.76966	104.14562	A1	22	0.00000
215	22	PHE	CE1	-40.30109	-22.30643	106.34948	A1	22	0.00000
216	22	PHE	CE2	-41.72224	-23.81970	105.04232	A1	22	0.00000
217	22	PHE	CZ	-40.86722	-23.58408	106.14281	A1	22	0.00000
218	22	PHE	C	-43.25845	-21.11988	101.58028	A1	22	0.00000
219	22	PHE	O	-44.19436	-20.32985	101.55111	A1	23	0.00000
220	23	MET	N	-43.39639	-22.43138	101.32298	A1	23	0.00000
221	23	MET	H	-42.59132	-23.03279	101.30500	A1	23	0.00000
222	23	MET	CA	-44.70480	-23.04357	101.02967	A1	23	0.00000
223	23	MET	CB	-45.08326	-22.73266	99.57140	A1	23	0.00000
224	23	MET	CG	-46.39952	-23.35273	99.09264	A1	23	0.00000
225	23	MET	SD	-46.67153	-23.10231	97.33272	A1	23	0.00000
226	23	MET	CE	-47.47592	-24.67640	96.98955	A1	23	0.00000
227	23	MET	C	-44.60710	-24.56281	101.21411	A1	23	0.00000
228	23	MET	O	-43.70841	-25.13566	100.62115	A1	23	0.00000
229	24	PHE	N	-45.43241	-25.30285	101.99622	A1	24	0.00000
230	24	PHE	H	-45.17063	-26.26850	102.03772	A1	24	0.00000
231	24	PHE	CA	-46.72021	-25.11140	102.69060	A1	24	0.00000
232	24	PHE	CB	-47.06193	-23.70552	103.21139	A1	24	0.00000
233	24	PHE	CG	-46.27878	-23.27691	104.43188	A1	24	0.00000
234	24	PHE	CD1	-46.28203	-24.06677	105.60532	A1	24	0.00000
235	24	PHE	CD2	-45.58233	-22.04683	104.40480	A1	24	0.00000
236	24	PHE	CE1	-45.58915	-23.62279	106.75356	A1	24	0.00000
237	24	PHE	CE2	-44.89083	-21.60100	105.55271	A1	24	0.00000
238	24	PHE	CZ	-44.89594	-22.39162	106.72434	A1	24	0.00000
239	24	PHE	C	-47.88569	-25.61775	101.85776	A1	24	0.00000
240	24	PHE	O	-48.73152	-24.87778	101.36424	A1	24	0.00000
241	25	ASP	N	-47.89055	-26.94593	101.74049	A1	25	0.00000
242	25	ASP	H	-47.22437	-27.52403	102.20704	A1	25	0.00000
243	25	ASP	CA	-48.86501	-27.64762	100.90165	A1	25	0.00000
244	25	ASP	CB	-48.21052	-27.81535	99.52046	A1	25	0.00000
245	25	ASP	CG	-49.19634	-28.30012	98.47932	A1	25	0.00000
246	25	ASP	OD1	-49.75750	-27.46672	97.77589	A1	25	0.00000
247	25	ASP	OD2	-49.39656	-29.50745	98.38197	A1	25	0.00000
248	25	ASP	C	-49.18430	-28.98699	101.56183	A1	25	0.00000
249	25	ASP	O	-48.57317	-29.35714	102.56241	A1	25	0.00000
250	26	PHE	N	-50.15819	-29.70261	101.00377	A1	26	0.00000
251	26	PHE	H	-50.60050	-29.39662	100.15349	A1	26	0.00000
252	26	PHE	CA	-50.56030	-30.99701	101.54898	A1	26	0.00000

FIG. 5

253	26	PHE	CB	51.42378	-30.83098	102.82009	A1	26	0.00000
254	26	PHE	CG	52.60356	-29.92038	102.57724	A1	26	0.00000
255	26	PHE	CD1	-52.50398	-28.55674	102.91777	A1	26	0.00000
256	26	PHE	CD2	-53.70380	-30.42265	101.99011	A1	26	0.00000
257	26	PHE	CE1	-53.58477	-27.68701	102.66706	A1	26	0.00000
258	26	PHE	CE2	-54.86474	-29.55076	101.74257	A1	26	0.00000
259	26	PHE	CZ	-54.76149	-28.18547	102.07912	A1	26	0.00000
260	26	PHE	C	-51.29340	-31.82500	100.51070	A1	26	0.00000
261	26	PHE	O	-51.63257	-31.38211	99.42184	A1	26	0.00000
262	27	ASP	N	-51.50640	-33.00225	100.89199	A1	27	0.00000
263	27	ASP	H	-51.30608	-33.34660	101.83544	A1	27	0.00000
264	27	ASP	CA	-52.05815	-34.11623	100.01741	A1	27	0.00000
265	27	ASP	CB	-53.56271	-34.25359	100.24733	A1	27	0.00000
266	27	ASP	CG	-53.82295	-35.66101	100.73899	A1	27	0.00000
267	27	ASP	OD1	-52.95640	-36.23164	101.40272	A1	27	0.00000
268	27	ASP	OD2	-54.89062	-36.19966	100.47314	A1	27	0.00000
269	27	ASP	C	-51.70102	-34.05698	98.54820	A1	27	0.00000
270	27	ASP	O	-52.51335	-34.10386	97.63254	A1	27	0.00000
271	28	GLY	N	-50.39045	-33.92246	98.35075	A1	28	0.00000
272	28	GLY	H	-49.78144	-33.80079	99.13160	A1	28	0.00000
273	28	GLY	CA	-49.88845	-33.86633	96.98221	A1	28	0.00000
274	28	GLY	C	-50.00090	-32.51821	96.28701	A1	28	0.00000
275	28	GLY	O	-49.04304	-32.03342	95.69731	A1	28	0.00000
276	29	ASP	N	-51.21573	-31.96145	96.33541	A1	29	0.00000
277	29	ASP	H	-51.93955	-32.39453	96.87595	A1	29	0.00000
278	29	ASP	CA	-51.52130	-30.85124	95.43198	A1	29	0.00000
279	29	ASP	CB	-52.38232	-31.44665	94.30287	A1	29	0.00000
280	29	ASP	CG	-52.46245	-30.54960	93.07981	A1	29	0.00000
281	29	ASP	OD1	-51.43429	-30.32445	92.44162	A1	29	0.00000
282	29	ASP	OD2	-53.56233	-30.10545	92.75048	A1	29	0.00000
283	29	ASP	C	-52.21461	-29.64631	96.07233	A1	29	0.00000
284	29	ASP	O	-52.39419	-28.59407	95.46732	A1	29	0.00000
285	30	GLU	N	-52.65130	-29.81701	97.32405	A1	30	0.00000
286	30	GLU	H	-52.34793	-30.57647	97.90251	A1	30	0.00000
287	30	GLU	CA	-53.43516	-28.70871	97.86160	A1	30	0.00000
288	30	GLU	CB	-54.71008	-29.18152	98.54724	A1	30	0.00000
289	30	GLU	CG	-55.84100	-29.71506	97.67444	A1	30	0.00000
290	30	GLU	CD	-57.13279	-29.50058	98.43828	A1	30	0.00000
291	30	GLU	OE1	-57.79466	-30.47326	98.78969	A1	30	0.00000
292	30	GLU	OE2	-57.48939	-28.34297	98.66447	A1	30	0.00000
293	30	GLU	C	-52.69655	-27.80995	98.82987	A1	30	0.00000
294	30	GLU	O	-52.13191	-28.20198	99.84476	A1	30	0.00000
295	31	ILE	N	-52.76110	-26.53268	98.46810	A1	31	0.00000
296	31	ILE	H	-53.28532	-26.29454	97.65353	A1	31	0.00000
297	31	ILE	CA	-51.98442	-25.52556	99.18511	A1	31	0.00000
298	31	ILE	CB	-51.81933	-24.32331	98.23317	A1	31	0.00000
299	31	ILE	CG2	-53.16329	-23.65625	97.91607	A1	31	0.00000
300	31	ILE	CG1	-50.75168	-23.33810	98.71478	A1	31	0.00000
301	31	ILE	CD	-50.41981	-22.27940	97.66271	A1	31	0.00000
302	31	ILE	C	-52.51316	-25.12446	100.56211	A1	31	0.00000
303	31	ILE	O	-53.70233	-24.97567	100.82175	A1	31	0.00000
304	32	PHE	N	-51.54696	-24.95576	101.46562	A1	32	0.00000
305	32	PHE	H	-50.59061	-25.06998	101.18020	A1	32	0.00000
306	32	PHE	CA	-51.85606	-24.57978	102.84494	A1	32	0.00000
307	32	PHE	CB	-50.76201	-25.18703	103.73391	A1	32	0.00000
308	32	PHE	CG	-51.19588	-26.22218	104.74893	A1	32	0.00000
309	32	PHE	CD1	-50.23927	-27.18148	105.15120	A1	32	0.00000
310	32	PHE	CD2	-52.49149	-26.22907	105.32111	A1	32	0.00000
311	32	PHE	CE1	-50.57386	-28.14516	106.12524	A1	32	0.00000
312	32	PHE	CE2	-52.82688	-27.19600	106.29575	A1	32	0.00000
313	32	PHE	CZ	-51.86606	-28.15152	106.69566	A1	32	0.00000
314	32	PHE	C	-51.84397	-23.07181	103.07985	A1	32	0.00000
315	32	PHE	O	-52.76581	-22.46086	103.62205	A1	32	0.00000
316	33	HIS	N	-50.69098	-22.30451	102.70813	A1	33	0.00000

FIG. 6

317	33	HIS	H	0.04312	-22.98834	102.10706	A1	33	0.00000
318	33	HIS	CA	-50.22576	-21.21727	103.23242	A1	33	0.00000
319	33	HIS	CB	-49.65908	-21.51540	104.63303	A1	33	0.00000
320	33	HIS	CG	-49.22984	-20.32142	105.45366	A1	33	0.00000
321	33	HIS	ND1	-48.02826	-19.72793	105.37205	A1	33	0.00000
322	33	HIS	HD1	-47.28999	-19.92757	104.75923	A1	33	0.00000
323	33	HIS	CD2	-49.97214	-19.68828	106.45019	A1	33	0.00000
324	33	HIS	NE2	-49.20118	-18.70682	106.97086	A1	33	0.00000
325	33	HIS	CE1	-48.00110	-18.72654	106.30763	A1	33	0.00000
326	33	HIS	C	-49.11511	-20.78472	102.29629	A1	33	0.00000
327	33	HIS	O	-48.59725	-21.61206	101.55845	A1	34	0.00000
328	34	VAL	N	-48.74537	-19.50449	102.33695	A1	34	0.00000
329	34	VAL	H	-49.19429	-18.80802	102.90183	A1	34	0.00000
330	34	VAL	CA	-47.51776	-19.11490	101.64269	A1	34	0.00000
331	34	VAL	CB	-47.81303	-18.42567	100.28392	A1	34	0.00000
332	34	VAL	CG1	-46.56686	-18.41158	99.39158	A1	34	0.00000
333	34	VAL	CG2	-48.95871	-19.06363	99.49006	A1	34	0.00000
334	34	VAL	C	-46.79652	-18.14692	102.56509	A1	34	0.00000
335	34	VAL	O	-47.41849	-17.54298	103.42874	A1	35	0.00000
336	35	ASP	N	-45.47963	-18.03426	102.37666	A1	35	0.00000
337	35	ASP	H	-45.03039	-18.68906	101.76710	A1	35	0.00000
338	35	ASP	CA	-44.68799	-16.93300	102.93355	A1	35	0.00000
339	35	ASP	CB	-44.74876	-15.73492	101.94639	A1	35	0.00000
340	35	ASP	CG	-46.11850	-15.06364	101.88569	A1	35	0.00000
341	35	ASP	OD1	-46.85196	-15.31279	100.93528	A1	35	0.00000
342	35	ASP	OD2	-46.43780	-14.28565	102.78747	A1	35	0.00000
343	35	ASP	C	-44.90949	-16.57120	104.41152	A1	35	0.00000
344	35	ASP	O	-45.03306	-17.43137	105.27733	A1	36	0.00000
345	36	MET	N	-44.91212	-15.26386	104.68945	A1	36	0.00000
346	36	MET	H	-44.97503	-14.58792	103.95356	A1	36	0.00000
347	36	MET	CA	-45.05621	-14.74244	106.04065	A1	36	0.00000
348	36	MET	CB	-44.58443	-13.28473	106.01845	A1	36	0.00000
349	36	MET	CG	-43.15122	-13.10955	105.50403	A1	36	0.00000
350	36	MET	SD	-42.96722	-11.71848	104.37016	A1	36	0.00000
351	36	MET	CE	-43.60204	-10.40582	105.42531	A1	36	0.00000
352	36	MET	C	-46.49207	-14.77022	106.53712	A1	36	0.00000
353	36	MET	O	-46.75425	-14.73983	107.73458	A1	37	0.00000
354	37	ALA	N	-47.43476	-14.70996	105.58618	A1	37	0.00000
355	37	ALA	H	-47.21869	-14.87225	104.60519	A1	37	0.00000
356	37	ALA	CA	-48.80100	-14.57493	106.05297	A1	37	0.00000
357	37	ALA	CB	-49.30059	-13.19637	105.61316	A1	37	0.00000
358	37	ALA	C	-49.83252	-15.61256	105.65673	A1	37	0.00000
359	37	ALA	O	-49.85254	-16.18787	104.57639	A1	38	0.00000
360	38	LYS	N	-50.76933	-15.79391	106.59397	A1	38	0.00000
361	38	LYS	H	-50.65212	-15.37866	107.49351	A1	38	0.00000
362	38	LYS	CA	-52.00981	-16.48765	106.23832	A1	38	0.00000
363	38	LYS	CB	-52.90628	-16.55867	107.48308	A1	38	0.00000
364	38	LYS	CG	-52.41585	-17.40517	108.60236	A1	38	0.00000
365	38	LYS	CD	-53.40991	-18.62084	108.86903	A1	38	0.00000
366	38	LYS	CE	-53.42547	-19.66155	107.75111	A1	38	0.00000
367	38	LYS	NZ	-54.76503	-20.17861	107.56038	A1	38	0.00000
368	38	LYS	HZ1	-54.79226	-20.92377	106.83759	A1	38	0.00000
369	38	LYS	HZ2	-55.17879	-20.59510	108.44046	A1	38	0.00000
370	38	LYS	HZ3	-55.42747	-19.41621	107.27224	A1	38	0.00000
371	38	LYS	C	-52.74081	-15.73437	105.12989	A1	38	0.00000
372	38	LYS	O	-52.72521	-14.51209	105.10297	A1	39	0.00000
373	39	LYS	N	-53.35457	-16.44351	104.17702	A1	39	0.00000
374	39	LYS	H	-53.59774	-15.96113	103.33578	A1	39	0.00000
375	39	LYS	CA	-53.67982	-17.86931	104.22041	A1	39	0.00000
376	39	LYS	CB	-55.18971	-18.00506	104.55346	A1	39	0.00000
377	39	LYS	CG	-56.24681	-17.84030	103.42417	A1	39	0.00000
378	39	LYS	CD	-56.27039	-16.52580	102.62130	A1	39	0.00000
379	39	LYS	CE	-56.64532	-16.69161	101.13213	A1	39	0.00000
380	39	LYS	NZ	-55.66137	-17.54082	100.43802	A1	39	0.00000

FIG. 7

381	39	LYS	HZ1	55.95645	-18.54581	100.36313	A1	3	0.00000
382	39	LYS	HZ2	-55.39863	-17.26725	99.46103	A1	39	0.00000
383	39	LYS	HZ3	-54.72486	-17.51921	100.90690	A1	39	0.00000
384	39	LYS	C	-53.44423	-18.44283	102.84633	A1	39	0.00000
385	39	LYS	O	-53.43351	-17.67518	101.88936	A1	39	0.00000
386	40	GLU	N	-53.41332	-19.77420	102.71885	A1	40	0.00000
387	40	GLU	H	-53.16154	-20.43691	103.42697	A1	40	0.00000
388	40	GLU	CA	-54.08892	-20.14645	101.48663	A1	40	0.00000
389	40	GLU	CB	-53.22132	-20.84643	100.44056	A1	40	0.00000
390	40	GLU	CG	-52.68203	-19.82757	99.41114	A1	40	0.00000
391	40	GLU	CD	-53.78227	-18.90107	98.89631	A1	40	0.00000
392	40	GLU	OE1	-53.60681	-17.68372	98.89245	A1	40	0.00000
393	40	GLU	OE2	-54.88246	-19.35560	98.59153	A1	40	0.00000
394	40	GLU	C	-55.46625	-20.74566	101.61501	A1	40	0.00000
395	40	GLU	O	-56.42031	-20.18304	101.08479	A1	40	0.00000
396	41	THR	N	-55.56321	-21.84976	102.35754	A1	41	0.00000
397	41	THR	H	-54.77319	-22.20472	102.86321	A1	41	0.00000
398	41	THR	CA	-56.84476	-22.55464	102.30963	A1	41	0.00000
399	41	THR	CB	-56.55011	-24.05030	102.16109	A1	41	0.00000
400	41	THR	OG1	-57.73042	-24.75407	101.74066	A1	41	0.00000
401	41	THR	HG1	-57.47835	-25.59614	101.33840	A1	41	0.00000
402	41	THR	CG2	-55.95304	-24.67173	103.43152	A1	41	0.00000
403	41	THR	C	-57.85722	-22.26510	103.42344	A1	41	0.00000
404	41	THR	O	-57.54877	-21.93546	104.56718	A1	41	0.00000
405	42	VAL	N	-59.12316	-22.41525	103.00455	A1	42	0.00000
406	42	VAL	H	-59.25687	-22.81422	102.09633	A1	42	0.00000
407	42	VAL	CA	-60.29134	-22.03291	103.80812	A1	42	0.00000
408	42	VAL	CB	-61.57611	-22.26846	102.98525	A1	42	0.00000
409	42	VAL	CG1	-62.83989	-21.83994	103.74041	A1	42	0.00000
410	42	VAL	CG2	-61.49852	-21.55078	101.63610	A1	42	0.00000
411	42	VAL	C	-60.39368	-22.75550	105.14170	A1	42	0.00000
412	42	VAL	O	-60.54018	-22.16641	106.20404	A1	43	0.00000
413	43	TRP	N	-60.26652	-24.07997	105.07466	A1	43	0.00000
414	43	TRP	H	-60.09540	-24.53437	104.20145	A1	43	0.00000
415	43	TRP	CA	-60.35178	-24.82113	106.34002	A1	43	0.00000
416	43	TRP	CB	-60.91225	-26.25321	106.17013	A1	43	0.00000
417	43	TRP	CG	-60.96314	-26.72606	104.73262	A1	43	0.00000
418	43	TRP	CD2	-59.88712	-27.12198	103.92127	A1	43	0.00000
419	43	TRP	CE2	-60.47947	-27.49629	102.60102	A1	43	0.00000
420	43	TRP	CE3	-58.50029	-27.24274	104.12574	A1	43	0.00000
421	43	TRP	CD1	-62.11826	-26.86040	103.93459	A1	43	0.00000
422	43	TRP	NE1	-61.84174	-27.31306	102.67766	A1	43	0.00000
423	43	TRP	HE1	-62.50030	-27.49046	101.97106	A1	43	0.00000
424	43	TRP	CZ2	-59.62565	-27.96652	101.58525	A1	43	0.00000
425	43	TRP	CZ3	-57.69263	-27.72260	103.07694	A1	43	0.00000
426	43	TRP	CH2	-58.24204	-28.07937	101.82597	A1	43	0.00000
427	43	TRP	C	-59.07150	-24.84373	107.16564	A1	43	0.00000
428	43	TRP	O	-58.85050	-25.68073	108.02836	A1	44	0.00000
429	44	ARG	N	-58.22471	-23.84563	106.89519	A1	44	0.00000
430	44	ARG	H	-58.31398	-23.27977	106.07364	A1	44	0.00000
431	44	ARG	CA	-57.22046	-23.49560	107.89144	A1	44	0.00000
432	44	ARG	CB	-55.83244	-23.69727	107.26013	A1	44	0.00000
433	44	ARG	CG	-54.63741	-23.63473	108.22026	A1	44	0.00000
434	44	ARG	CD	-53.30915	-23.64273	107.47006	A1	44	0.00000
435	44	ARG	NE	-52.18625	-23.26000	108.32672	A1	44	0.00000
436	44	ARG	HE	-52.36221	-22.91543	109.25139	A1	44	0.00000
437	44	ARG	CZ	-50.93149	-23.33650	107.86475	A1	44	0.00000
438	44	ARG	NH1	-49.92358	-22.86519	108.56844	A1	44	0.00000
439	44	ARG	HH11	-48.98076	-22.84912	108.24673	A1	44	0.00000
440	44	ARG	HH12	-50.05162	-22.52238	109.51721	A1	44	0.00000
441	44	ARG	NH2	-50.67215	-23.69024	106.69352	A1	44	0.00000
442	44	ARG	HH21	-49.73591	-23.96008	106.35139	A1	44	0.00000
443	44	ARG	HH22	-51.41769	-24.25918	106.14195	A1	44	0.00000
444	44	ARG	C	-57.42751	-22.95857	108.38029	A1	44	0.00000

FIG. 8

./DR1_MIN2.CRD Thu Feb 25 14:58:48 1993 8

445	44	ARG	O	6.53064	-21.39201	108.88943	A1	44	0.00000
446	45	LEU	N	-58.65270	-21.55686	108.18548	A1	45	0.00000
447	45	LEU	H	-59.36846	-22.06382	107.69729	A1	45	0.00000
448	45	LEU	CA	-58.94679	-20.21897	108.70611	A1	45	0.00000
449	45	LEU	CB	-59.87267	-19.46515	107.74942	A1	45	0.00000
450	45	LEU	CG	-59.15056	-18.96990	106.49579	A1	45	0.00000
451	45	LEU	CD1	-60.14534	-18.41906	105.47407	A1	45	0.00000
452	45	LEU	CD2	-58.10431	-17.92289	106.87944	A1	45	0.00000
453	45	LEU	C	-59.55818	-20.20104	110.09168	A1	45	0.00000
454	45	LEU	O	-59.53362	-19.19926	110.79199	A1	45	0.00000
455	46	GLU	N	-60.08917	-21.36024	110.48954	A1	46	0.00000
456	46	GLU	H	-60.14047	-22.14708	109.87631	A1	46	0.00000
457	46	GLU	CA	-60.58379	-21.47317	111.86481	A1	46	0.00000
458	46	GLU	CB	-61.47817	-22.71518	111.95437	A1	46	0.00000
459	46	GLU	CG	-60.80881	-24.02305	111.51772	A1	46	0.00000
460	46	GLU	CD	-61.85264	-25.11830	111.46594	A1	46	0.00000
461	46	GLU	OE1	-62.26867	-25.47222	110.36424	A1	46	0.00000
462	46	GLU	OE2	-62.24894	-25.60616	112.52280	A1	46	0.00000
463	46	GLU	C	-59.48698	-21.49323	112.92683	A1	46	0.00000
464	46	GLU	O	-59.60959	-21.22226	114.10493	A1	46	0.00000
465	47	GLU	N	-58.27888	-21.79310	112.44220	A1	47	0.00000
466	47	GLU	H	-58.18142	-22.06659	111.48920	A1	47	0.00000
467	47	GLU	CA	-57.08155	-21.73864	113.27698	A1	47	0.00000
468	47	GLU	CB	-55.89121	-22.09481	112.39059	A1	47	0.00000
469	47	GLU	CG	-55.95036	-23.50661	111.78977	A1	47	0.00000
470	47	GLU	CD	-55.55418	-24.58648	112.78701	A1	47	0.00000
471	47	GLU	OE1	-55.48886	-25.74409	112.37878	A1	47	0.00000
472	47	GLU	OE2	-55.29749	-24.27876	113.95212	A1	47	0.00000
473	47	GLU	C	-56.83827	-20.38151	113.91510	A1	47	0.00000
474	47	GLU	O	-56.67000	-19.35742	113.26194	A1	47	0.00000
475	48	PHE	N	-56.83807	-20.40716	115.24713	A1	48	0.00000
476	48	PHE	H	-56.92233	-21.28123	115.72305	A1	48	0.00000
477	48	PHE	CA	-56.75617	-19.13647	115.96362	A1	48	0.00000
478	48	PHE	CB	-57.20231	-19.34982	117.41420	A1	48	0.00000
479	48	PHE	CG	-58.41697	-18.49841	117.70829	A1	48	0.00000
480	48	PHE	CD1	-59.71122	-19.00320	117.44215	A1	48	0.00000
481	48	PHE	CD2	-58.25459	-17.19966	118.24455	A1	48	0.00000
482	48	PHE	CE1	-60.84630	-18.20670	117.71246	A1	48	0.00000
483	48	PHE	CE2	-59.38940	-16.40286	118.51469	A1	48	0.00000
484	48	PHE	CZ	-60.68202	-16.90878	118.24779	A1	48	0.00000
485	48	PHE	C	-55.39240	-18.46628	115.93777	A1	48	0.00000
486	48	PHE	O	-54.35117	-19.07618	115.72587	A1	48	0.00000
487	49	GLY	N	-55.43214	-17.15361	116.19781	A1	49	0.00000
488	49	GLY	H	-56.32069	-16.72101	116.34575	A1	49	0.00000
489	49	GLY	CA	-54.23420	-16.30520	116.13162	A1	49	0.00000
490	49	GLY	C	-52.92695	-16.86464	116.68056	A1	49	0.00000
491	49	GLY	O	-51.85815	-16.69886	116.10714	A1	49	0.00000
492	50	ARG	N	-53.03915	-17.56211	117.81779	A1	50	0.00000
493	50	ARG	H	-53.93666	-17.67284	118.24069	A1	50	0.00000
494	50	ARG	CA	-51.84656	-18.16800	118.42224	A1	50	0.00000
495	50	ARG	CB	-52.27437	-18.92760	119.68340	A1	50	0.00000
496	50	ARG	CG	-51.10260	-19.32736	120.58254	A1	50	0.00000
497	50	ARG	CD	-51.53002	-20.14774	121.80047	A1	50	0.00000
498	50	ARG	NE	-50.37432	-20.44943	122.64580	A1	50	0.00000
499	50	ARG	HE	-49.69865	-19.71957	122.75767	A1	50	0.00000
500	50	ARG	CZ	-50.24449	-21.63184	123.26571	A1	50	0.00000
501	50	ARG	NH1	-49.18578	-21.84466	124.04503	A1	50	0.00000
502	50	ARG	HH11	-49.05579	-22.71179	124.52612	A1	50	0.00000
503	50	ARG	HH12	-48.49360	-21.13233	124.16453	A1	50	0.00000
504	50	ARG	NH2	-51.15926	-22.58629	123.10623	A1	50	0.00000
505	50	ARG	HH21	-51.08073	-23.47414	123.56513	A1	50	0.00000
506	50	ARG	HH22	-51.95092	-22.42795	122.51852	A1	50	0.00000
507	50	ARG	C	-51.06703	-19.09561	117.49074	A1	50	0.00000
508	50	ARG	O	-49.84240	-19.09133	117.41926	A1	50	0.00000

FIG. 9

509	51	PHE	N	[illegible]	-19.87778	116.73839	A1	51	0.00000
510	51	PHE	H	-52.84564	-19.76657	116.76797	A1	51	0.00000
511	51	PHE	CA	-51.29477	-20.78796	115.73402	A1	51	0.00000
512	51	PHE	CB	-52.51672	-21.52503	115.15449	A1	51	0.00000
513	51	PHE	CG	-52.25099	-22.49194	114.02359	A1	51	0.00000
514	51	PHE	CD1	-51.87888	-23.82851	114.29503	A1	51	0.00000
515	51	PHE	CD2	-52.45788	-22.06484	112.69289	A1	51	0.00000
516	51	PHE	CE1	-51.72483	-24.74421	113.22969	A1	51	0.00000
517	51	PHE	CE2	-52.30778	-22.98082	111.63059	A1	51	0.00000
518	51	PHE	CZ	-51.94314	-24.31860	111.90000	A1	51	0.00000
519	51	PHE	C	-50.50268	-20.00696	114.69371	A1	51	0.00000
520	51	PHE	O	-49.31281	-20.20801	114.47961	A1	51	0.00000
521	52	ALA	N	-51.20469	-19.03212	114.10202	A1	52	0.00000
522	52	ALA	H	-52.16823	-18.89764	114.33870	A1	52	0.00000
523	52	ALA	CA	-50.54896	-18.16486	113.11957	A1	52	0.00000
524	52	ALA	CB	-51.52058	-17.09216	112.62511	A1	52	0.00000
525	52	ALA	C	-49.28257	-17.48933	113.62687	A1	52	0.00000
526	52	ALA	O	-48.27008	-17.39834	112.94510	A1	52	0.00000
527	53	SER	N	-49.35763	-17.04955	114.88764	A1	53	0.00000
528	53	SER	H	-50.22411	-17.11498	115.38567	A1	53	0.00000
529	53	SER	CA	-48.18100	-16.47055	115.53815	A1	53	0.00000
530	53	SER	CB	-48.58146	-16.02158	116.95383	A1	53	0.00000
531	53	SER	OG	-47.59593	-15.15541	117.52845	A1	53	0.00000
532	53	SER	HG	-47.05158	-14.90357	118.42105	A1	53	0.00000
533	53	SER	C	-46.99433	-17.42737	115.57426	A1	53	0.00000
534	53	SER	O	-45.89463	-17.11790	115.12568	A1	53	0.00000
535	54	PHE	N	-47.26082	-18.64220	116.08200	A1	54	0.00000
536	54	PHE	H	-48.18040	-18.87361	116.41568	A1	54	0.00000
537	54	PHE	CA	-46.18727	-19.64350	116.09999	A1	54	0.00000
538	54	PHE	CB	-46.69548	-20.99079	116.63413	A1	54	0.00000
539	54	PHE	CG	-46.90625	-20.99411	118.13255	A1	54	0.00000
540	54	PHE	CD1	-48.11656	-21.50316	118.65539	A1	54	0.00000
541	54	PHE	CD2	-45.89246	-20.53119	119.00621	A1	54	0.00000
542	54	PHE	CE1	-48.31310	-21.55376	120.05266	A1	54	0.00000
543	54	PHE	CE2	-46.08993	-20.57973	120.40382	A1	54	0.00000
544	54	PHE	CZ	-47.30008	-21.09192	120.92307	A1	54	0.00000
545	54	PHE	C	-45.57270	-19.90650	114.73758	A1	54	0.00000
546	54	PHE	O	-44.36030	-19.93109	114.55246	A1	54	0.00000
547	55	GLU	N	-46.46681	-20.08976	113.76558	A1	55	0.00000
548	55	GLU	H	-47.45338	-20.04226	113.95516	A1	55	0.00000
549	55	GLU	CA	-45.97322	-20.41545	112.42886	A1	55	0.00000
550	55	GLU	CB	-47.14512	-20.81915	111.54876	A1	55	0.00000
551	55	GLU	CG	-47.92567	-21.96126	112.19274	A1	55	0.00000
552	55	GLU	CD	-49.04456	-22.36202	111.27677	A1	55	0.00000
553	55	GLU	OE1	-49.15553	-23.53977	110.96047	A1	55	0.00000
554	55	GLU	OE2	-49.80524	-21.50984	110.81474	A1	55	0.00000
555	55	GLU	C	-45.19354	-19.30188	111.76318	A1	55	0.00000
556	55	GLU	O	-44.12678	-19.50387	111.19343	A1	55	0.00000
557	56	ALA	N	-45.73650	-18.08673	111.89532	A1	56	0.00000
558	56	ALA	H	-46.62336	-17.96765	112.34890	A1	56	0.00000
559	56	ALA	CA	-45.00414	-16.92733	111.38640	A1	56	0.00000
560	56	ALA	CB	-45.80074	-15.63871	111.59969	A1	56	0.00000
561	56	ALA	C	-43.63772	-16.77849	112.02791	A1	56	0.00000
562	56	ALA	O	-42.62065	-16.60634	111.36878	A1	57	0.00000
563	57	GLN	N	-43.63088	-16.91454	113.35929	A1	57	0.00000
564	57	GLN	H	-44.48826	-17.03983	113.86832	A1	57	0.00000
565	57	GLN	CA	-42.35063	-16.88200	114.06847	A1	57	0.00000
566	57	GLN	CB	-42.61987	-17.03049	115.56930	A1	57	0.00000
567	57	GLN	CG	-41.40659	-16.75355	116.45895	A1	57	0.00000
568	57	GLN	CD	-41.80070	-16.94589	117.90800	A1	57	0.00000
569	57	GLN	OE1	-42.29879	-16.06206	118.58910	A1	57	0.00000
570	57	GLN	NE2	-41.55425	-18.16011	118.38366	A1	57	0.00000
571	57	GLN	HE21	-41.14709	-18.27176	117.81428	A1	57	0.00000
572	57	GLN	HE22	-41.78115	-18.36728	119.33313	A1	57	0.00000

FIG. 10

./DR1_MIN2.CRD Thu Feb 25 14:58:48 1993 10

573	57	GLN	C	1.36213	-17.94055	113.59025	A1	57	0.00000
574	57	GLN	O	-40.18971	-17.68051	113.34773	A1	57	0.00000
575	58	GLY	N	-41.88825	-19.15742	113.41319	A1	58	0.00000
576	58	GLY	H	-42.84771	-19.33514	113.64847	A1	58	0.00000
577	58	GLY	CA	-41.05379	-20.23393	112.87374	A1	58	0.00000
578	58	GLY	C	-40.45534	-19.92781	111.50957	A1	58	0.00000
579	58	GLY	O	-39.25324	-20.01021	111.27849	A1	58	0.00000
580	59	ALA	N	-41.34654	-19.52227	110.60018	A1	59	0.00000
581	59	ALA	H	-42.32072	-19.46762	110.83485	A1	59	0.00000
582	59	ALA	CA	-40.88666	-19.14537	109.26181	A1	59	0.00000
583	59	ALA	CB	-42.07124	-18.74086	108.30101	A1	59	0.00000
584	59	ALA	C	-39.86090	-18.02257	109.26073	A1	59	0.00000
585	59	ALA	O	-38.85187	-18.04905	108.56603	A1	60	0.00000
586	60	LEU	N	-40.12979	-17.02925	110.11113	A1	60	0.00000
587	60	LEU	H	-40.96678	-17.03715	110.66448	A1	60	0.00000
588	60	LEU	CA	-39.17026	-15.93079	110.21454	A1	60	0.00000
589	60	LEU	CB	-39.82974	-14.72108	110.88234	A1	60	0.00000
590	60	LEU	CG	-41.00342	-14.16448	110.06267	A1	60	0.00000
591	60	LEU	CD1	-41.72077	-13.05637	110.83175	A1	60	0.00000
592	60	LEU	CD2	-40.54968	-13.69403	108.67852	A1	60	0.00000
593	60	LEU	C	-37.86300	-16.28607	110.90549	A1	60	0.00000
594	60	LEU	O	-36.81366	-15.71151	110.64266	A1	60	0.00000
595	61	ALA	N	-37.92548	-17.30628	111.76650	A1	61	0.00000
596	61	ALA	H	-38.80416	-17.70206	112.04737	A1	61	0.00000
597	61	ALA	CA	-36.66060	-17.86080	112.25036	A1	61	0.00000
598	61	ALA	CB	-36.90091	-18.87147	113.37402	A1	61	0.00000
599	61	ALA	C	-35.86652	-18.52303	111.13575	A1	61	0.00000
600	61	ALA	O	-34.67753	-18.28483	110.93578	A1	61	0.00000
601	62	ASN	N	-36.59182	-19.33011	110.35468	A1	62	0.00000
602	62	ASN	H	-37.55651	-19.52444	110.56458	A1	62	0.00000
603	62	ASN	CA	-35.93048	-19.97053	109.20954	A1	62	0.00000
604	62	ASN	CB	-36.90608	-20.83397	108.41185	A1	62	0.00000
605	62	ASN	CG	-36.14296	-21.97501	107.76767	A1	62	0.00000
606	62	ASN	OD1	-35.90083	-23.00051	108.38915	A1	62	0.00000
607	62	ASN	ND2	-35.81296	-21.80385	106.49294	A1	62	0.00000
608	62	ASN	HD21	-35.71613	-20.90910	106.04169	A1	62	0.00000
609	62	ASN	HD22	-35.64736	-22.62041	105.92778	A1	62	0.00000
610	62	ASN	C	-35.27272	-18.97317	108.27635	A1	62	0.00000
611	62	ASN	O	-34.08977	-19.05772	107.98073	A1	63	0.00000
612	63	ILE	N	-36.07385	-17.96130	107.91224	A1	63	0.00000
613	63	ILE	H	-37.03805	-17.97906	108.18770	A1	63	0.00000
614	63	ILE	CA	-35.60960	-16.86395	107.05550	A1	63	0.00000
615	63	ILE	CB	-36.79680	-15.88630	106.84927	A1	63	0.00000
616	63	ILE	CG2	-36.71800	-14.58751	107.66300	A1	63	0.00000
617	63	ILE	CG1	-37.00443	-15.60068	105.36486	A1	63	0.00000
618	63	ILE	CD	-38.27181	-14.79756	105.06416	A1	63	0.00000
619	63	ILE	C	-34.32421	-16.14412	107.48562	A1	63	0.00000
620	63	ILE	O	-33.67028	-15.43835	106.72047	A1	64	0.00000
621	64	ALA	N	-33.97867	-16.34078	108.76481	A1	64	0.00000
622	64	ALA	H	-34.55914	-16.88095	109.37800	A1	64	0.00000
623	64	ALA	CA	-32.68252	-15.86370	109.23001	A1	64	0.00000
624	64	ALA	CB	-32.78414	-15.37252	110.67448	A1	64	0.00000
625	64	ALA	C	-31.59324	-16.91956	109.13883	A1	64	0.00000
626	64	ALA	O	-30.45701	-16.65389	108.75412	A1	65	0.00000
627	65	VAL	N	-31.96250	-18.15367	109.50633	A1	65	0.00000
628	65	VAL	H	-32.92093	-18.37377	109.71401	A1	65	0.00000
629	65	VAL	CA	-30.91507	-19.17596	109.47932	A1	65	0.00000
630	65	VAL	CB	-31.28412	-20.41152	110.33210	A1	65	0.00000
631	65	VAL	CG1	-31.53866	-19.97521	111.77524	A1	65	0.00000
632	65	VAL	CG2	-32.45603	-21.23819	109.79675	A1	65	0.00000
633	65	VAL	C	-30.45713	-19.56758	108.08237	A1	65	0.00000
634	65	VAL	O	-29.26568	-19.71596	107.82437	A1	66	0.00000
635	66	ASP	N	-31.42136	-19.66027	107.15805	A1	66	0.00000
636	66	ASP	H	-32.38553	-19.49723	107.38832	A1	66	0.00000

FIG. 11

./DAC_MAIN2.CRD Tue Feb 25 14:58:48 1993 13

637	66	ASP	CA	1.04858	-19.93216	105.76795	A1	66	0.00000
638	66	ASP	CB	-32.31036	-20.24966	104.93007	A1	66	0.00000
639	66	ASP	CG	-33.44297	-19.24219	105.08208	A1	66	0.00000
640	66	ASP	OD1	-33.16986	-18.05114	105.20729	A1	66	0.00000
641	66	ASP	OD2	-34.60286	-19.65468	105.08126	A1	66	0.00000
642	66	ASP	C	-30.18178	-18.83449	105.15564	A1	66	0.00000
643	66	ASP	O	-29.16482	-19.06872	104.50705	A1	66	0.00000
644	67	LYS	N	-30.56424	-17.59916	105.48017	A1	67	0.00000
645	67	LYS	H	-31.49538	-17.48655	105.84055	A1	67	0.00000
646	67	LYS	CA	-29.72959	-16.43204	105.19320	A1	67	0.00000
647	67	LYS	CB	-30.39071	-15.23196	105.87104	A1	67	0.00000
648	67	LYS	CG	-29.79159	-13.86177	105.56853	A1	67	0.00000
649	67	LYS	CD	-30.51506	-12.79056	106.38164	A1	67	0.00000
650	67	LYS	CE	-29.96446	-11.38645	106.14720	A1	67	0.00000
651	67	LYS	NZ	-30.60526	-10.44891	107.01869	A1	67	0.00000
652	67	LYS	HZ1	-30.33262	-9.48398	106.85909	A1	67	0.00000
653	67	LYS	HZ2	-31.70143	-10.49161	106.80064	A1	67	0.00000
654	67	LYS	HZ3	-30.53221	-10.71804	108.01156	A1	67	0.00000
655	67	LYS	C	-28.28117	-16.58093	105.64383	A1	67	0.00000
656	67	LYS	O	-27.33559	-16.44078	104.87661	A1	67	0.00000
657	68	ALA	N	-28.12520	-16.92373	106.92795	A1	68	0.00000
658	68	ALA	H	-28.92119	-17.00935	107.53692	A1	68	0.00000
659	68	ALA	CA	-26.76352	-17.18143	107.40958	A1	68	0.00000
660	68	ALA	CB	-26.77377	-17.44846	108.91534	A1	68	0.00000
661	68	ALA	C	-26.07149	-18.34364	106.70618	A1	68	0.00000
662	68	ALA	O	-24.80989	-18.33297	106.37143	A1	68	0.00000
663	69	ASN	N	-26.87877	-19.37475	106.44973	A1	69	0.00000
664	69	ASN	H	-27.84416	-19.34421	106.72158	A1	69	0.00000
665	69	ASN	CA	-26.32826	-20.54731	105.77098	A1	69	0.00000
666	69	ASN	CB	-27.33794	-21.70567	105.74618	A1	69	0.00000
667	69	ASN	CG	-27.75534	-22.20215	107.12937	A1	69	0.00000
668	69	ASN	OD1	-28.81753	-22.77967	107.30600	A1	69	0.00000
669	69	ASN	ND2	-26.90880	-21.98927	108.13718	A1	69	0.00000
670	69	ASN	HD21	-26.02949	-21.53117	108.03476	A1	69	0.00000
671	69	ASN	HD22	-27.17968	-22.29754	109.04652	A1	69	0.00000
672	69	ASN	C	-25.83413	-20.26827	104.36379	A1	69	0.00000
673	69	ASN	O	-24.88019	-20.87816	103.89106	A1	69	0.00000
674	70	LEU	N	-26.46696	-19.27268	103.71664	A1	70	0.00000
675	70	LEU	H	-27.27121	-18.83110	104.12686	A1	70	0.00000
676	70	LEU	CA	-25.93555	-18.80513	102.42930	A1	70	0.00000
677	70	LEU	CB	-26.70466	-17.57714	101.93156	A1	70	0.00000
678	70	LEU	CG	-28.07464	-17.87907	101.32608	A1	70	0.00000
679	70	LEU	CD1	-28.90878	-16.60756	101.23109	A1	70	0.00000
680	70	LEU	CD2	-27.93286	-18.56192	99.96378	A1	70	0.00000
681	70	LEU	C	-24.47328	-18.42736	102.51389	A1	70	0.00000
682	70	LEU	O	-23.64160	-18.86456	101.72791	A1	70	0.00000
683	71	GLU	N	-24.17065	-17.62592	103.54240	A1	71	0.00000
684	71	GLU	H	-24.87529	-17.33320	104.19342	A1	71	0.00000
685	71	GLU	CA	-22.77384	-17.24207	103.73624	A1	71	0.00000
686	71	GLU	CB	-22.68099	-16.23884	104.88750	A1	71	0.00000
687	71	GLU	CG	-21.33647	-15.50613	104.93364	A1	71	0.00000
688	71	GLU	CD	-21.30052	-14.53829	106.10023	A1	71	0.00000
689	71	GLU	OE1	-20.27115	-14.47665	106.76970	A1	71	0.00000
690	71	GLU	OE2	-22.29376	-13.85012	106.33423	A1	71	0.00000
691	71	GLU	C	-21.86369	-18.43808	103.97868	A1	71	0.00000
692	71	GLU	O	-20.81243	-18.61050	103.36820	A1	71	0.00000
693	72	ILE	N	-22.34609	-19.31836	104.86364	A1	72	0.00000
694	72	ILE	H	-23.21301	-19.12129	105.33200	A1	72	0.00000
695	72	ILE	CA	-21.56703	-20.53142	105.13649	A1	72	0.00000
696	72	ILE	CB	-22.29516	-21.40405	106.17923	A1	72	0.00000
697	72	ILE	CG2	-21.51796	-22.68646	106.50604	A1	72	0.00000
698	72	ILE	CG1	-22.55172	-20.59465	107.45409	A1	72	0.00000
699	72	ILE	CD	-23.34520	-21.36378	108.51180	A1	72	0.00000
700	72	ILE	C	-21.22106	-21.35113	103.89490	A1	72	0.00000

FIG. 12

701	72	ILE	O	20.06679	-21.68162	103.64178	A1	72 0.00000
702	73	MET	N	-22.24406	-21.67127	103.09738	A1	73 0.00000
703	73	MET	H	-23.17806	-21.34412	103.27303	A1	73 0.00000
704	73	MET	CA	-21.88577	-22.51146	101.95532	A1	73 0.00000
705	73	MET	CB	-23.02917	-23.44601	101.56487	A1	73 0.00000
706	73	MET	CG	-23.30745	-24.44882	102.69030	A1	73 0.00000
707	73	MET	SD	-24.39480	-25.79652	102.19686	A1	73 0.00000
708	73	MET	CE	-24.58745	-26.56731	103.81212	A1	73 0.00000
709	73	MET	C	-21.30840	-21.79430	100.75010	A1	73 0.00000
710	73	MET	O	-20.54740	-22.36938	99.97894	A1	73 0.00000
711	74	THR	N	-21.60342	-20.49214	100.63510	A1	74 0.00000
712	74	THR	H	-22.28955	-20.04403	101.21510	A1	74 0.00000
713	74	THR	CA	-20.82593	-19.73833	99.64704	A1	74 0.00000
714	74	THR	CB	-21.46299	-18.35496	99.36040	A1	74 0.00000
715	74	THR	OG1	-21.01301	-17.84761	98.09669	A1	74 0.00000
716	74	THR	HG1	-20.04699	-17.88381	98.02785	A1	74 0.00000
717	74	THR	CG2	-21.20740	-17.31089	100.44667	A1	74 0.00000
718	74	THR	C	-19.35170	-19.61359	100.02467	A1	74 0.00000
719	74	THR	O	-18.48554	-19.49348	99.16750	A1	74 0.00000
720	75	LYS	N	-19.08538	-19.69260	101.33717	A1	75 0.00000
721	75	LYS	H	-19.81875	-19.65220	102.02321	A1	75 0.00000
722	75	LYS	CA	-17.69833	-19.83955	101.77078	A1	75 0.00000
723	75	LYS	CB	-17.61408	-19.57287	103.27797	A1	75 0.00000
724	75	LYS	CG	-16.20208	-19.66153	103.86107	A1	75 0.00000
725	75	LYS	CD	-16.21091	-19.57437	105.38567	A1	75 0.00000
726	75	LYS	CE	-14.81504	-19.74395	105.98417	A1	75 0.00000
727	75	LYS	NZ	-14.91179	-19.69891	107.44939	A1	75 0.00000
728	75	LYS	HZ1	-13.96820	-19.83508	107.86470	A1	75 0.00000
729	75	LYS	HZ2	-15.29159	-18.77551	107.74094	A1	75 0.00000
730	75	LYS	HZ3	-15.54844	-20.45311	107.77639	A1	75 0.00000
731	75	LYS	C	-17.14118	-21.21778	101.45102	A1	75 0.00000
732	75	LYS	O	-16.11623	-21.36022	100.79660	A1	76 0.00000
733	76	ARG	N	-17.86151	-22.25466	101.90990	A1	76 0.00000
734	76	ARG	H	-18.69512	-22.09296	102.44436	A1	76 0.00000
735	76	ARG	CA	-17.35520	-23.61422	101.67525	A1	76 0.00000
736	76	ARG	CB	-18.33654	-24.68494	102.17145	A1	76 0.00000
737	76	ARG	CG	-18.82789	-24.66219	103.62361	A1	76 0.00000
738	76	ARG	CD	-19.55383	-25.98411	103.91795	A1	76 0.00000
739	76	ARG	NE	-20.36155	-25.99642	105.14334	A1	76 0.00000
740	76	ARG	HE	-21.34527	-25.85364	105.02467	A1	76 0.00000
741	76	ARG	CZ	-19.85069	-26.28686	106.34915	A1	76 0.00000
742	76	ARG	NH1	-20.67426	-26.45770	107.38550	A1	76 0.00000
743	76	ARG	HH11	-20.32038	-26.64144	108.30551	A1	76 0.00000
744	76	ARG	HH12	-21.67206	-26.42100	107.26619	A1	76 0.00000
745	76	ARG	NH2	-18.53304	-26.41209	106.51158	A1	76 0.00000
746	76	ARG	HH21	-18.12377	-26.62371	107.39854	A1	76 0.00000
747	76	ARG	HH22	-17.92942	-26.29542	105.72237	A1	76 0.00000
748	76	ARG	C	-17.06072	-23.91761	100.20901	A1	76 0.00000
749	76	ARG	O	-16.02715	-24.45819	99.83552	A1	77 0.00000
750	77	SER	N	-18.01091	-23.50462	99.36716	A1	77 0.00000
751	77	SER	H	-18.84286	-23.05363	99.69917	A1	77 0.00000
752	77	SER	CA	-17.80506	-23.71642	97.93702	A1	77 0.00000
753	77	SER	CB	-19.13837	-24.15898	97.32351	A1	77 0.00000
754	77	SER	OG	-18.92403	-25.08061	96.24728	A1	77 0.00000
755	77	SER	HG	-18.99574	-24.62840	95.39572	A1	77 0.00000
756	77	SER	C	-17.22854	-22.51234	97.20137	A1	77 0.00000
757	77	SER	O	-17.39865	-22.33993	96.00106	A1	78 0.00000
758	78	ASN	N	-16.52714	-21.66944	97.97646	A1	78 0.00000
759	78	ASN	H	-16.44843	-21.84082	98.96113	A1	78 0.00000
760	78	ASN	CA	-15.74721	-20.53857	97.45264	A1	78 0.00000
761	78	ASN	CB	-14.33390	-21.01377	97.09195	A1	78 0.00000
762	78	ASN	CG	-13.52905	-21.21984	98.36114	A1	78 0.00000
763	78	ASN	OD1	-12.89966	-20.31632	98.89264	A1	78 0.00000
764	78	ASN	ND2	-13.55264	-22.45457	98.85326	A1	78 0.00000

FIG. 13

765	78	ASN	HD21	4.08412	-23.19170	98.43678	A1	78	0.00000
766	78	ASN	HD22	-13.03871	-22.65362	99.68493	A1	78	0.00000
767	78	ASN	C	-16.34134	-19.72172	96.31352	A1	78	0.00000
768	78	ASN	O	-15.71478	-19.42979	95.30178	A1	78	0.00000
769	79	TYR	N	-17.59612	-19.32597	96.52354	A1	79	0.00000
770	79	TYR	H	-18.05424	-19.55771	97.38252	A1	79	0.00000
771	79	TYR	CA	-18.21408	-18.48918	95.49858	A1	79	0.00000
772	79	TYR	CB	-19.64874	-18.92649	95.21260	A1	79	0.00000
773	79	TYR	CG	-19.74485	-20.32764	94.65360	A1	79	0.00000
774	79	TYR	CD1	-20.64246	-21.23278	95.25950	A1	79	0.00000
775	79	TYR	CE1	-20.76017	-22.54189	94.75217	A1	79	0.00000
776	79	TYR	CD2	-18.96361	-20.72112	93.54108	A1	79	0.00000
777	79	TYR	CE2	-19.07884	-22.03339	93.03642	A1	79	0.00000
778	79	TYR	CZ	-19.97533	-22.93822	93.64752	A1	79	0.00000
779	79	TYR	OH	-20.07585	-24.23438	93.18578	A1	79	0.00000
780	79	TYR	HH	-19.67682	-24.30670	92.31232	A1	79	0.00000
781	79	TYR	C	-18.21035	-17.01261	95.83719	A1	79	0.00000
782	79	TYR	O	-18.85099	-16.51273	96.76683	A1	79	0.00000
783	80	THR	N	-17.42457	-16.33235	95.00452	A1	80	0.00000
784	80	THR	H	-16.96429	-16.79509	94.24288	A1	80	0.00000
785	80	THR	CA	-17.09577	-14.92660	95.20513	A1	80	0.00000
786	80	THR	CB	-15.89072	-14.87711	96.18098	A1	80	0.00000
787	80	THR	OG1	-15.49849	-13.52440	96.43537	A1	80	0.00000
788	80	THR	HG1	-14.60960	-13.50159	96.80560	A1	80	0.00000
789	80	THR	CG2	-14.69719	-15.72265	95.72104	A1	80	0.00000
790	80	THR	C	-16.77512	-14.32258	93.03840	A1	80	0.00000
791	80	THR	O	-16.16879	-14.97644	92.99811	A1	80	0.00000
792	81	PRO	N	-17.23243	-13.08096	93.61451	A1	81	0.00000
793	81	PRO	CD	-18.04687	-12.25452	94.50529	A1	81	0.00000
794	81	PRO	CA	-16.95963	-12.43774	92.32255	A1	81	0.00000
795	81	PRO	CB	-18.08102	-11.39225	92.28996	A1	81	0.00000
796	81	PRO	CG	-18.22970	-10.94901	93.74456	A1	81	0.00000
797	81	PRO	C	-15.57247	-11.80328	92.25040	A1	81	0.00000
798	81	PRO	O	-15.41926	-10.58936	92.16776	A1	81	0.00000
799	82	ILE	N	-14.55883	-12.66988	92.27154	A1	82	0.00000
800	82	ILE	H	-14.69364	-13.66392	92.31920	A1	82	0.00000
801	82	ILE	CA	-13.18946	-12.18130	92.13921	A1	82	0.00000
802	82	ILE	CB	-12.60010	-11.87598	93.53959	A1	82	0.00000
803	82	ILE	CG2	-12.41140	-13.13773	94.38674	A1	82	0.00000
804	82	ILE	CG1	-11.31152	-11.05228	93.44331	A1	82	0.00000
805	82	ILE	CD	-10.76554	-10.62709	94.80896	A1	82	0.00000
806	82	ILE	C	-12.35649	-13.19907	91.37376	A1	82	0.00000
807	82	ILE	OCT1	-11.36717	-12.81747	90.75062	A1	82	0.00000
808	82	ILE	OCT2	-12.72556	-14.37446	91.38671	A1	82	0.00000
809	83	GLY	N	-17.53322	-0.31236	94.99084	B1	1	0.00000
810	83	GLY	HT1	-17.21994	0.44323	94.35235	B1	1	0.00000
811	83	GLY	HT2	-16.86357	-1.12219	94.96444	B1	1	0.00000
812	83	GLY	HT3	-17.61098	0.01920	95.97150	B1	1	0.00000
813	83	GLY	CA	-18.79853	-0.91116	94.55151	B1	1	0.00000
814	83	GLY	C	-18.62573	-2.38203	94.66351	B1	1	0.00000
815	83	GLY	O	-17.35786	-2.70920	94.84086	B1	1	0.00000
816	84	ASP	N	-19.57260	-3.20239	94.59303	B1	2	0.00000
817	84	ASP	H	-20.49658	-2.89510	94.35600	B1	2	0.00000
818	84	ASP	CA	-19.43900	-4.63200	94.86181	B1	2	0.00000
819	84	ASP	CB	-19.44643	-4.83356	96.38475	B1	2	0.00000
820	84	ASP	CG	-18.89301	-6.19619	96.73815	B1	2	0.00000
821	84	ASP	OD1	-17.69451	-6.29764	96.98109	B1	2	0.00000
822	84	ASP	OD2	-19.66566	-7.14958	96.75715	B1	2	0.00000
823	84	ASP	C	-20.62786	-5.31072	94.19848	B1	2	0.00000
824	84	ASP	O	-21.46903	-4.61697	93.63479	B1	2	0.00000
825	85	THR	N	-20.67796	-6.64606	94.24891	B1	3	0.00000
826	85	THR	H	-20.04362	-7.15926	94.84032	B1	3	0.00000
827	85	THR	CA	-21.75257	-7.39367	93.59154	B1	3	0.00000
828	85	THR	CB	-21.58903	-7.31950	92.05122	B1	3	0.00000

FIG. 14

829	85	THR	OG1	22.76265	-7.82480	91.39964	B1	3	0.00000
830	85	THR	HG1	-22.73431	-7.60152	90.46343	B1	3	0.00000
831	85	THR	CG2	-20.32966	-8.02078	91.53071	B1	3	0.00000
832	85	THR	C	-21.74290	-8.83241	94.09035	B1	3	0.00000
833	85	THR	O	-20.76454	-9.30377	94.65381	B1	3	0.00000
834	86	ARG	N	-22.86491	-9.52779	93.88799	B1	4	0.00000
835	86	ARG	H	-23.62404	-9.13760	93.36423	B1	4	0.00000
836	86	ARG	CA	-22.93360	-10.87552	94.44830	B1	4	0.00000
837	86	ARG	CB	-23.51668	-10.79083	95.86916	B1	4	0.00000
838	86	ARG	CG	-22.74323	-11.65365	96.87092	B1	4	0.00000
839	86	ARG	CD	-23.23116	-13.10294	97.02541	B1	4	0.00000
840	86	ARG	NE	-22.12580	-14.03911	97.27083	B1	4	0.00000
841	86	ARG	HE	-21.93083	-14.68836	96.53494	B1	4	0.00000
842	86	ARG	CZ	-21.37502	-14.05016	98.38612	B1	4	0.00000
843	86	ARG	NH1	-20.31371	-14.85617	98.44757	B1	4	0.00000
844	86	ARG	HH11	-19.73815	-14.87872	99.26299	B1	4	0.00000
845	86	ARG	HH12	-20.05194	-15.47498	97.69021	B1	4	0.00000
846	86	ARG	NH2	-21.67517	-13.26636	99.42563	B1	4	0.00000
847	86	ARG	HH21	-21.13780	-13.26659	100.26897	B1	4	0.00000
848	86	ARG	HH22	-22.46145	-12.65025	99.36831	B1	4	0.00000
849	86	ARG	C	-23.73522	-11.82065	93.57905	B1	4	0.00000
850	86	ARG	O	-24.85200	-11.52803	93.17882	B1	4	0.00000
851	87	PRO	N	-23.12190	-12.98532	93.27325	B1	5	0.00000
852	87	PRO	CD	-21.73269	-13.34562	93.54376	B1	5	0.00000
853	87	PRO	CA	-23.84439	-14.02757	92.53087	B1	5	0.00000
854	87	PRO	CB	-22.78528	-15.13066	92.39999	B1	5	0.00000
855	87	PRO	CG	-21.43460	-14.43376	92.52460	B1	5	0.00000
856	87	PRO	C	-25.10390	-14.54496	93.21975	B1	5	0.00000
857	87	PRO	O	-25.32441	-14.39544	94.41838	B1	5	0.00000
858	88	ARG	N	-25.94344	-15.17061	92.39123	B1	6	0.00000
859	88	ARG	H	-25.68611	-15.35588	91.44433	B1	6	0.00000
860	88	ARG	CA	-27.23219	-15.62675	92.90235	B1	6	0.00000
861	88	ARG	CB	-28.29078	-15.39805	91.81653	B1	6	0.00000
862	88	ARG	CG	-29.70863	-15.55859	92.35844	B1	6	0.00000
863	88	ARG	CD	-30.79150	-14.91787	91.49236	B1	6	0.00000
864	88	ARG	NE	-31.92741	-14.57277	92.34607	B1	6	0.00000
865	88	ARG	HE	-31.76512	-14.64038	93.33788	B1	6	0.00000
866	88	ARG	CZ	-33.08881	-14.12165	91.86193	B1	6	0.00000
867	88	ARG	NH1	-34.06565	-13.81756	92.71322	B1	6	0.00000
868	88	ARG	HH11	-34.95441	-13.48197	92.40144	B1	6	0.00000
869	88	ARG	HH12	-33.91853	-13.92533	93.69838	B1	6	0.00000
870	88	ARG	NH2	-33.26623	-13.97383	90.54974	B1	6	0.00000
871	88	ARG	HH21	-34.12737	-13.64013	90.16725	B1	6	0.00000
872	88	ARG	HH22	-32.52080	-14.19859	89.92214	B1	6	0.00000
873	88	ARG	C	-27.23157	-17.07404	93.36366	B1	6	0.00000
874	88	ARG	O	-26.89591	-18.00090	92.63574	B1	6	0.00000
875	89	PHE	N	-27.62757	-17.24057	94.62546	B1	7	0.00000
876	89	PHE	H	-27.92346	-16.46797	95.18173	B1	7	0.00000
877	89	PHE	CA	-27.64368	-18.59443	95.17433	B1	7	0.00000
878	89	PHE	CB	-26.56379	-18.74887	96.25427	B1	7	0.00000
879	89	PHE	CG	-25.20774	-18.55805	95.61829	B1	7	0.00000
880	89	PHE	CD1	-24.74915	-19.48139	94.64858	B1	7	0.00000
881	89	PHE	CD2	-24.42840	-17.43023	95.96102	B1	7	0.00000
882	89	PHE	CE1	-23.51045	-19.27079	94.00961	B1	7	0.00000
883	89	PHE	CE2	-23.18767	-17.21976	95.32384	B1	7	0.00000
884	89	PHE	CZ	-22.73800	-18.13927	94.34976	B1	7	0.00000
885	89	PHE	C	-28.99632	-18.97147	95.72084	B1	7	0.00000
886	89	PHE	O	-29.85551	-18.12429	95.94786	B1	7	0.00000
887	90	LEU	N	-29.15750	-20.28822	95.87791	B1	8	0.00000
888	90	LEU	H	-28.38720	-20.92114	95.76376	B1	8	0.00000
889	90	LEU	CA	-30.48975	-20.82226	96.14113	B1	8	0.00000
890	90	LEU	CB	-31.01268	-21.46546	94.84981	B1	8	0.00000
891	90	LEU	CG	-32.46079	-21.16892	94.43614	B1	8	0.00000
892	90	LEU	CD1	-32.81137	-21.98230	93.19113	B1	8	0.00000

FIG. 15

./DR1_MIN2.CRD Thu Feb 25 14:58:48 1993 15

893	90	LEU	CD2	3.47498	-21.40699	95.55222	B1	8	0.00000
894	90	LEU	C	-30.45467	-21.90281	97.20252	B1	8	0.00000
895	90	LEU	O	-29.74216	-22.89200	97.07224	B1	8	0.00000
896	91	TRP	N	-31.28133	-21.71086	98.22982	B1	9	0.00000
897	91	TRP	H	-31.78897	-20.85226	98.31900	B1	9	0.00000
898	91	TRP	CA	-31.61477	-22.86043	99.06700	B1	9	0.00000
899	91	TRP	CB	-31.76159	-22.50789	100.54418	B1	9	0.00000
900	91	TRP	CG	-30.46050	-22.11490	101.18157	B1	9	0.00000
901	91	TRP	CD2	-29.22893	-22.79283	101.16170	B1	9	0.00000
902	91	TRP	CE2	-28.30074	-21.96546	101.98847	B1	9	0.00000
903	91	TRP	CE3	-28.77368	-24.00327	100.60389	B1	9	0.00000
904	91	TRP	CD1	-30.26500	-20.96427	101.96112	B1	9	0.00000
905	91	TRP	NE1	-28.99810	-20.87047	102.44030	B1	9	0.00000
906	91	TRP	HE1	-28.68566	-20.15616	103.04137	B1	9	0.00000
907	91	TRP	CZ2	-26.97767	-22.40520	102.16578	B1	9	0.00000
908	91	TRP	CZ3	-27.44054	-24.40402	100.81577	B1	9	0.00000
909	91	TRP	CH2	-26.56124	-23.61859	101.58828	B1	9	0.00000
910	91	TRP	C	-32.96765	-23.39534	98.70806	B1	9	0.00000
911	91	TRP	O	-33.92486	-22.66026	98.49798	B1	9	0.00000
912	92	GLN	N	-33.02847	-24.71550	98.69197	B1	10	0.00000
913	92	GLN	H	-32.20362	-25.28365	98.76579	B1	10	0.00000
914	92	GLN	CA	-34.33516	-25.34751	98.65309	B1	10	0.00000
915	92	GLN	CB	-34.50105	-26.04119	97.30049	B1	10	0.00000
916	92	GLN	CG	-34.43287	-25.05724	96.13126	B1	10	0.00000
917	92	GLN	CD	-34.12668	-25.79390	94.84833	B1	10	0.00000
918	92	GLN	OE1	-32.99424	-25.88838	94.39010	B1	10	0.00000
919	92	GLN	NE2	-35.19268	-26.32196	94.25873	B1	10	0.00000
920	92	GLN	HE21	-36.10617	-26.21874	94.65013	B1	10	0.00000
921	92	GLN	HE22	-35.08609	-26.83019	93.40658	B1	10	0.00000
922	92	GLN	C	-34.37000	-26.35610	99.77327	B1	10	0.00000
923	92	GLN	O	-33.40619	-27.07419	100.00960	B1	10	0.00000
924	93	LEU	N	-35.49484	-26.39205	100.47380	B1	11	0.00000
925	93	LEU	H	-36.24432	-25.74963	100.29272	B1	11	0.00000
926	93	LEU	CA	-35.59559	-27.43909	101.48633	B1	11	0.00000
927	93	LEU	CB	-35.41178	-26.81504	102.88181	B1	11	0.00000
928	93	LEU	CG	-34.83577	-27.70766	103.99848	B1	11	0.00000
929	93	LEU	CD1	-34.33031	-26.83824	105.14843	B1	11	0.00000
930	93	LEU	CD2	-35.82812	-28.74167	104.52005	B1	11	0.00000
931	93	LEU	C	-36.93596	-28.11112	101.32695	B1	11	0.00000
932	93	LEU	O	-37.91692	-27.47571	100.96621	B1	11	0.00000
933	94	LYS	N	-36.95045	-29.41719	101.56549	B1	12	0.00000
934	94	LYS	H	-36.10205	-29.89066	101.79736	B1	12	0.00000
935	94	LYS	CA	-38.21063	-30.14121	101.49214	B1	12	0.00000
936	94	LYS	CB	-38.26049	-30.88530	100.13839	B1	12	0.00000
937	94	LYS	CG	-39.43761	-31.85442	100.07544	B1	12	0.00000
938	94	LYS	CD	-39.91969	-32.44832	98.75113	B1	12	0.00000
939	94	LYS	CE	-41.00198	-33.40442	99.23924	B1	12	0.00000
940	94	LYS	NZ	-41.98389	-33.90963	98.26846	B1	12	0.00000
941	94	LYS	HZ1	-42.69798	-34.41995	98.86351	B1	12	0.00000
942	94	LYS	HZ2	-42.49249	-33.14263	97.78947	B1	12	0.00000
943	94	LYS	HZ3	-41.57162	-34.57937	97.59540	B1	12	0.00000
944	94	LYS	C	-38.34910	-31.08699	102.67642	B1	12	0.00000
945	94	LYS	O	-37.54720	-31.99770	102.85849	B1	12	0.00000
946	95	PHE	N	-39.40676	-30.85929	103.46609	B1	13	0.00000
947	95	PHE	H	-39.99321	-30.05201	103.34519	B1	13	0.00000
948	95	PHE	CA	-39.73794	-31.84982	104.49053	B1	13	0.00000
949	95	PHE	CB	-39.13251	-31.49228	105.86481	B1	13	0.00000
950	95	PHE	CG	-39.62104	-30.20819	106.49960	B1	13	0.00000
951	95	PHE	CD1	-39.04917	-28.96886	106.12996	B1	13	0.00000
952	95	PHE	CD2	-40.60068	-30.26479	107.51173	B1	13	0.00000
953	95	PHE	CE1	-39.45587	-27.78326	106.77985	B1	13	0.00000
954	95	PHE	CE2	-41.01477	-29.08019	108.16313	B1	13	0.00000
955	95	PHE	CZ	-40.43557	-27.84435	107.79605	B1	13	0.00000
956	95	PHE	C	-41.22005	-32.16799	104.57423	B1	13	0.00000

FIG. 16

./DR1_MDM2.CRD Thu Feb 25 14:58:48 1993 16

957	95	PHE	O	- .08591	-31.31332	104.41691	B1	13	-0.00000
958	96	GLU	N	-44.47812	-33.46734	104.75822	B1	14	0.00000
959	96	GLU	H	-40.74093	-34.09071	105.01948	B1	14	0.00000
960	96	GLU	CA	-42.80002	-33.99059	104.40078	B1	14	0.00000
961	96	GLU	CB	-42.75085	-34.25375	102.88321	B1	14	0.00000
962	96	GLU	CG	-43.92070	-34.87965	102.11791	B1	14	0.00000
963	96	GLU	CD	-43.55505	-34.92496	100.64018	B1	14	0.00000
964	96	GLU	OE1	-44.08205	-34.15253	99.84297	B1	14	0.00000
965	96	GLU	OE2	-42.67962	-35.68559	100.23154	B1	14	0.00000
966	96	GLU	C	-43.13129	-35.25393	105.17925	B1	14	0.00000
967	96	GLU	O	-42.27510	-36.11395	105.37879	B1	14	0.00000
968	97	CYS	N	-44.39621	-35.34431	105.62501	B1	15	0.00000
969	97	CYS	H	-45.05281	-34.60566	105.44206	B1	15	0.00000
970	97	CYS	CA	-44.78990	-36.60747	106.25700	B1	15	0.00000
971	97	CYS	CB	-45.09404	-36.46870	107.76554	B1	15	0.00000
972	97	CYS	SG	-46.49873	-35.54248	108.42288	B1	15	0.00000
973	97	CYS	C	-45.89248	-37.36966	105.55706	B1	15	0.00000
974	97	CYS	O	-46.75253	-36.80546	104.88787	B1	15	0.00000
975	98	HIS	N	-45.80356	-38.69951	105.71784	B1	16	0.00000
976	98	HIS	H	-45.06854	-39.11332	106.26371	B1	16	0.00000
977	98	HIS	CA	-46.75592	-39.59530	105.05785	B1	16	0.00000
978	98	HIS	CB	-46.00867	-40.61029	104.19437	B1	16	0.00000
979	98	HIS	CG	-45.38253	-39.98357	102.97364	B1	16	0.00000
980	98	HIS	ND1	-45.88967	-40.13539	101.74183	B1	16	0.00000
981	98	HIS	HD1	-46.72307	-40.60043	101.51181	B1	16	0.00000
982	98	HIS	CD2	-44.21286	-39.22166	102.89430	B1	16	0.00000
983	98	HIS	NE2	-44.02278	-38.92334	101.58753	B1	16	0.00000
984	98	HIS	CE1	-45.05268	-39.48082	100.87633	B1	16	0.00000
985	98	HIS	C	-47.56750	-40.40062	106.05217	B1	16	0.00000
986	98	HIS	O	-47.04279	-40.99638	106.99225	B1	16	0.00000
987	99	PHE	N	-48.87987	-40.39547	105.81218	B1	17	0.00000
988	99	PHE	H	-49.25243	-39.92869	105.00666	B1	17	0.00000
989	99	PHE	CA	-49.78029	-41.01889	106.77662	B1	17	0.00000
990	99	PHE	CB	-50.48946	-39.93190	107.59234	B1	17	0.00000
991	99	PHE	CG	-49.63868	-39.72312	108.81497	B1	17	0.00000
992	99	PHE	CD1	-48.50685	-38.87580	108.76543	B1	17	0.00000
993	99	PHE	CD2	-49.92563	-40.47457	109.97439	B1	17	0.00000
994	99	PHE	CE1	-47.64103	-38.80002	109.87537	B1	17	0.00000
995	99	PHE	CE2	-49.06252	-40.39779	111.08354	B1	17	0.00000
996	99	PHE	CZ	-47.92137	-39.56658	111.02626	B1	17	0.00000
997	99	PHE	C	-50.79242	-41.97404	106.19800	B1	17	0.00000
998	99	PHE	O	-51.48007	-41.71068	105.22101	B1	18	0.00000
999	100	PHE	N	-50.86837	-43.12653	106.85844	B1	18	0.00000
1000	100	PHE	H	-50.32768	-43.27017	107.68944	B1	18	0.00000
1001	100	PHE	CA	-51.84718	-44.10783	106.41132	B1	18	0.00000
1002	100	PHE	CB	-51.44468	-45.52210	106.04262	B1	18	0.00000
1003	100	PHE	CG	-51.08740	-46.34931	105.63001	B1	18	0.00000
1004	100	PHE	CD1	-49.81159	-46.95065	105.55366	B1	18	0.00000
1005	100	PHE	CD2	-52.01269	-46.50158	104.56911	B1	18	0.00000
1006	100	PHE	CE1	-49.45012	-47.69723	104.41336	B1	18	0.00000
1007	100	PHE	CE2	-51.65494	-47.24829	103.42719	B1	18	0.00000
1008	100	PHE	CZ	-50.37408	-47.83859	103.35608	B1	18	0.00000
1009	100	PHE	C	-53.21727	-43.84401	106.96975	B1	18	0.00000
1010	100	PHE	O	-53.38235	-43.49692	108.13319	B1	18	0.00000
1011	101	ASN	N	-54.19611	-44.08275	106.08672	B1	19	0.00000
1012	101	ASN	H	-53.92777	-44.28429	105.14366	B1	19	0.00000
1013	101	ASN	CA	-55.63451	-43.97453	106.37273	B1	19	0.00000
1014	101	ASN	CB	-56.35400	-45.03359	105.52094	B1	19	0.00000
1015	101	ASN	CG	-57.86040	-44.83624	105.52911	B1	19	0.00000
1016	101	ASN	OD1	-58.43246	-44.06601	104.77523	B1	19	0.00000
1017	101	ASN	ND2	-58.51327	-45.58184	106.41359	B1	19	0.00000
1018	101	ASN	HD21	-58.04843	-46.21753	107.02623	B1	19	0.00000
1019	101	ASN	HD22	-59.50666	-45.49785	106.46882	B1	19	0.00000
1020	101	ASN	C	-56.06277	-44.09262	107.83398	B1	19	0.00000

FIG. 17

./DA1_NEW2.CRD Thu Feb 25 14:58:48 1993 17

1021	101	ASN	O	-56.73737	-43.23997	108.39463	B1	19	0.00000
1022	102	GLY	N	-55.63460	-45.10941	108.46454	B1	20	0.00000
1023	102	GLY	H	-55.00370	-45.02188	108.01935	B1	20	0.00000
1024	102	GLY	CA	-55.97438	-45.32353	109.88157	B1	20	0.00000
1025	102	GLY	C	-55.02088	-44.59872	110.81953	B1	20	0.00000
1026	102	GLY	O	-54.46008	-45.17864	111.73800	B1	21	0.00000
1027	103	THR	N	-54.84744	-43.29716	110.54648	B1	21	0.00000
1028	103	THR	H	-55.35512	-42.90731	109.77435	B1	21	0.00000
1029	103	THR	CA	-53.96549	-42.39542	111.30363	B1	21	0.00000
1030	103	THR	CB	-54.75487	-41.81263	112.51011	B1	21	0.00000
1031	103	THR	OG1	-54.22405	-40.53356	112.87483	B1	21	0.00000
1032	103	THR	HG1	-54.81974	-40.09919	113.49221	B1	21	0.00000
1033	103	THR	CG2	-54.86925	-42.72433	113.73959	B1	21	0.00000
1034	103	THR	C	-52.56983	-42.92386	111.66956	B1	21	0.00000
1035	103	THR	O	-51.96086	-42.59288	112.68707	B1	22	0.00000
1036	104	GLU	N	-52.05837	-43.78433	110.78327	B1	22	0.00000
1037	104	GLU	H	-52.50836	-43.94021	109.90068	B1	22	0.00000
1038	104	GLU	CA	-50.80234	-44.42458	111.16198	B1	22	0.00000
1039	104	GLU	CB	-50.88647	-45.95191	111.05395	B1	22	0.00000
1040	104	GLU	CG	-51.13368	-46.62525	112.41591	B1	22	0.00000
1041	104	GLU	CD	-50.07267	-46.21410	113.43075	B1	22	0.00000
1042	104	GLU	OE1	-50.42273	-45.91599	114.57130	B1	22	0.00000
1043	104	GLU	OE2	-48.89658	-46.13148	113.08359	B1	22	0.00000
1044	104	GLU	C	-49.56607	-43.91901	110.45954	B1	22	0.00000
1045	104	GLU	O	-49.58628	-43.40196	109.34894	B1	23	0.00000
1046	105	ARG	N	-48.46470	-44.04978	111.19345	B1	23	0.00000
1047	105	ARG	H	-48.46820	-44.67995	111.97754	B1	23	0.00000
1048	105	ARG	CA	-47.23862	-43.36578	110.79677	B1	23	0.00000
1049	105	ARG	CB	-46.43619	-43.14957	112.09184	B1	23	0.00000
1050	105	ARG	CG	-45.11167	-42.37595	112.05228	B1	23	0.00000
1051	105	ARG	CD	-43.89570	-43.22016	111.65081	B1	23	0.00000
1052	105	ARG	NE	-42.65640	-42.48704	111.89499	B1	23	0.00000
1053	105	ARG	HE	-42.30777	-42.45915	112.83941	B1	23	0.00000
1054	105	ARG	CZ	-42.05554	-41.77685	110.93892	B1	23	0.00000
1055	105	ARG	NH1	-41.02352	-41.00938	111.25165	B1	23	0.00000
1056	105	ARG	HH11	-40.51476	-40.49136	110.56874	B1	23	0.00000
1057	105	ARG	HH12	-40.73208	-40.92747	112.21979	B1	23	0.00000
1058	105	ARG	NH2	-42.47661	-41.82718	109.68286	B1	23	0.00000
1059	105	ARG	HH21	-42.19810	-41.15340	109.00310	B1	23	0.00000
1060	105	ARG	HH22	-43.08503	-42.57763	109.38941	B1	23	0.00000
1061	105	ARG	C	-46.47373	-44.13883	109.74376	B1	23	0.00000
1062	105	ARG	O	-46.02105	-45.25363	109.97034	B1	23	0.00000
1063	106	VAL	N	-46.32883	-43.51517	108.56827	B1	24	0.00000
1064	106	VAL	H	-46.72693	-42.61352	108.37187	B1	24	0.00000
1065	106	VAL	CA	-45.53349	-44.24499	107.58352	B1	24	0.00000
1066	106	VAL	CB	-46.27081	-44.39073	106.24298	B1	24	0.00000
1067	106	VAL	CG1	-45.79579	-45.65575	105.52366	B1	24	0.00000
1068	106	VAL	CG2	-47.77990	-44.41166	106.42922	B1	24	0.00000
1069	106	VAL	C	-44.14065	-43.66075	107.41554	B1	24	0.00000
1070	106	VAL	O	-43.30354	-43.80891	108.29696	B1	24	0.00000
1071	107	ARG	N	-43.87314	-42.98069	106.29416	B1	25	0.00000
1072	107	ARG	H	-44.58452	-42.69040	105.65671	B1	25	0.00000
1073	107	ARG	CA	-42.49561	-42.53115	106.12329	B1	25	0.00000
1074	107	ARG	CB	-41.95685	-43.01317	104.76032	B1	25	0.00000
1075	107	ARG	CG	-41.96328	-42.02619	103.58362	B1	25	0.00000
1076	107	ARG	CD	-42.33357	-42.66829	102.24883	B1	25	0.00000
1077	107	ARG	NE	-43.76838	-42.93515	102.23147	B1	25	0.00000
1078	107	ARG	HE	-44.37946	-42.14312	102.28284	B1	25	0.00000
1079	107	ARG	CZ	-44.26510	-44.17490	102.20945	B1	25	0.00000
1080	107	ARG	NH1	-45.56598	-44.32747	102.35905	B1	25	0.00000
1081	107	ARG	HH11	-46.00629	-45.19207	102.34562	B1	25	0.00000
1082	107	ARG	HH12	-46.19539	-43.55730	102.54612	B1	25	0.00000
1083	107	ARG	NH2	-43.47983	-45.23695	102.05798	B1	25	0.00000
1084	107	ARG	HH21	-43.86541	-46.15996	102.05452	B1	25	0.00000

FIG. 18

./CAL_KDH2.CRD Thu Feb 25 14:58:48 1993 18

1085	107	ARG	HH22	2.49404	-45.11997	101.94496	B1	25	0.00000
1086	107	ARG	C	-42.37787	-41.03546	106.32504	B1	25	0.00000
1087	107	ARG	O	-43.36896	-40.31981	106.43645	B1	25	0.00000
1088	108	LEU	N	-41.12633	-40.58602	106.39627	B1	26	0.00000
1089	108	LEU	H	-40.32617	-41.17985	106.29320	B1	26	0.00000
1090	108	LEU	CA	-40.89942	-39.15744	106.53751	B1	26	0.00000
1091	108	LEU	CB	-40.80087	-38.80954	108.01248	B1	26	0.00000
1092	108	LEU	CG	-41.96347	-37.89689	108.35874	B1	26	0.00000
1093	108	LEU	CD1	-42.75820	-38.44729	109.53808	B1	26	0.00000
1094	108	LEU	CD2	-41.50070	-36.44650	108.50151	B1	26	0.00000
1095	108	LEU	C	-39.62061	-38.77273	105.85764	B1	26	0.00000
1096	108	LEU	O	-38.76368	-39.61093	105.60154	B1	26	0.00000
1097	109	LEU	N	-39.52150	-37.47828	105.56773	B1	27	0.00000
1098	109	LEU	H	-40.28459	-36.84167	105.72467	B1	27	0.00000
1099	109	LEU	CA	-38.30683	-37.02679	104.90334	B1	27	0.00000
1100	109	LEU	CB	-38.47418	-37.24039	103.39009	B1	27	0.00000
1101	109	LEU	CG	-39.74490	-36.59695	102.82634	B1	27	0.00000
1102	109	LEU	CD1	-39.42210	-35.25631	102.17066	B1	27	0.00000
1103	109	LEU	CD2	-40.49190	-37.56523	101.91138	B1	27	0.00000
1104	109	LEU	C	-37.99969	-35.58061	105.21268	B1	27	0.00000
1105	109	LEU	O	-38.88411	-34.77322	105.47943	B1	27	0.00000
1106	110	GLU	N	-36.70092	-35.29768	105.12126	B1	28	0.00000
1107	110	GLU	H	-36.01498	-36.01786	105.00992	B1	28	0.00000
1108	110	GLU	CA	-36.20315	-33.92985	105.08184	B1	28	0.00000
1109	110	GLU	CB	-35.80977	-33.47627	106.49578	B1	28	0.00000
1110	110	GLU	CG	-35.32216	-32.02210	106.60993	B1	28	0.00000
1111	110	GLU	CD	-33.83808	-31.87178	106.30413	B1	28	0.00000
1112	110	GLU	OE1	-33.37957	-30.74951	106.10521	B1	28	0.00000
1113	110	GLU	OE2	-33.09671	-32.85201	106.36491	B1	28	0.00000
1114	110	GLU	C	-35.01026	-33.94076	104.15500	B1	28	0.00000
1115	110	GLU	O	-34.25577	-34.90807	104.11585	B1	28	0.00000
1116	111	ARG	N	-34.89439	-32.86843	103.37222	B1	29	0.00000
1117	111	ARG	H	-35.61365	-32.16766	103.37387	B1	29	0.00000
1118	111	ARG	CA	-33.75645	-32.74903	102.46249	B1	29	0.00000
1119	111	ARG	CB	-33.99004	-33.60407	101.20352	B1	29	0.00000
1120	111	ARG	CG	-35.45106	-33.70037	100.75305	B1	29	0.00000
1121	111	ARG	CD	-35.67880	-34.83036	99.75174	B1	29	0.00000
1122	111	ARG	NE	-37.09124	-35.21147	99.72614	B1	29	0.00000
1123	111	ARG	HE	-37.71860	-34.61357	100.22757	B1	29	0.00000
1124	111	ARG	CZ	-37.50098	-36.32384	99.09789	B1	29	0.00000
1125	111	ARG	NH1	-38.78116	-36.68971	99.16119	B1	29	0.00000
1126	111	ARG	HH11	-39.12269	-37.49888	98.68276	B1	29	0.00000
1127	111	ARG	HH12	-39.43712	-36.16699	99.70940	B1	29	0.00000
1128	111	ARG	NH2	-36.63391	-37.06893	98.41518	B1	29	0.00000
1129	111	ARG	HH21	-36.91501	-37.90348	97.94325	B1	29	0.00000
1130	111	ARG	HH22	-35.67503	-36.78688	98.36264	B1	29	0.00000
1131	111	ARG	C	-33.49135	-31.31194	102.08170	B1	29	0.00000
1132	111	ARG	O	-34.39395	-30.54569	101.76699	B1	29	0.00000
1133	112	CYS	N	-32.20568	-30.97057	102.12414	B1	30	0.00000
1134	112	CYS	H	-31.50733	-31.64380	102.37455	B1	30	0.00000
1135	112	CYS	CA	-31.80468	-29.62360	101.73826	B1	30	0.00000
1136	112	CYS	CB	-31.12874	-28.92365	102.91930	B1	30	0.00000
1137	112	CYS	SG	-30.70297	-27.19555	102.57697	B1	30	0.00000
1138	112	CYS	C	-30.87388	-29.64998	100.54380	B1	30	0.00000
1139	112	CYS	O	-29.97769	-30.48052	100.40406	B1	30	0.00000
1140	113	ILE	N	-31.15975	-28.70696	99.65078	B1	31	0.00000
1141	113	ILE	H	-31.84193	-28.00116	99.86111	B1	31	0.00000
1142	113	ILE	CA	-30.55306	-28.70228	98.32464	B1	31	0.00000
1143	113	ILE	CB	-31.56021	-29.33526	97.30706	B1	31	0.00000
1144	113	ILE	CG2	-33.00339	-29.37434	97.82323	B1	31	0.00000
1145	113	ILE	CG1	-31.52431	-28.74184	95.89635	B1	31	0.00000
1146	113	ILE	CD	-32.44047	-29.50025	94.93272	B1	31	0.00000
1147	113	ILE	C	-30.08576	-27.29665	97.96536	B1	31	0.00000
1148	113	ILE	O	-30.75333	-26.29900	98.21317	B1	31	0.00000

FIG. 19

1149	114	TYR	N	28.87010	-27.25564	97.41665	B1	32	0.00000
1150	114	TYR	H	-28.42970	-28.10151	97.10297	D1	32	0.00000
1151	114	TYR	CA	-28.22036	-25.98264	97.11462	B1	32	0.00000
1152	114	TYR	CB	-26.80088	-26.01933	97.71345	B1	32	0.00000
1153	114	TYR	CG	-26.01127	-24.72107	97.61311	B1	32	0.00000
1154	114	TYR	CD1	-26.62770	-23.45825	97.79068	B1	32	0.00000
1155	114	TYR	CE1	-25.84886	-22.28083	97.75267	B1	32	0.00000
1156	114	TYR	CD2	-24.61824	-24.80211	97.38751	B1	32	0.00000
1157	114	TYR	CE2	-23.83841	-23.62651	97.34588	B1	32	0.00000
1158	114	TYR	CZ	-24.45600	-22.36940	97.53154	B1	32	0.00000
1159	114	TYR	OH	-23.68967	-21.21917	97.50979	B1	32	0.00000
1160	114	TYR	HH	-22.79676	-21.43015	97.21984	B1	32	0.00000
1161	114	TYR	C	-28.14723	-25.83215	95.61430	B1	32	0.00000
1162	114	TYR	O	-27.66375	-26.70965	94.91236	B1	32	0.00000
1163	115	ASN	N	-28.66823	-24.69995	95.12919	B1	33	0.00000
1164	115	ASN	H	-29.03092	-24.02391	95.77643	B1	33	0.00000
1165	115	ASN	CA	-28.63762	-24.41545	93.68566	B1	33	0.00000
1166	115	ASN	CB	-27.27049	-23.84385	93.27078	B1	33	0.00000
1167	115	ASN	CG	-27.00239	-22.43118	93.78440	B1	33	0.00000
1168	115	ASN	OD1	-26.55389	-22.16954	94.85370	B1	33	0.00000
1169	115	ASN	ND2	-27.51765	-21.48359	92.96271	B1	33	0.00000
1170	115	ASN	HD21	-28.04883	-21.70692	92.14797	B1	33	0.00000
1171	115	ASN	HD22	-27.29503	-20.52370	93.13946	B1	33	0.00000
1172	115	ASN	C	-28.96318	-25.59300	92.77321	B1	33	0.00000
1173	115	ASN	O	-28.22150	-25.91402	91.85250	B1	33	0.00000
1174	116	GLN	N	-30.10691	-26.23583	93.07767	B1	34	0.00000
1175	116	GLN	H	-30.66790	-25.92614	93.84830	B1	34	0.00000
1176	116	GLN	CA	-30.60575	-27.38897	92.31212	B1	34	0.00000
1177	116	GLN	CB	-30.73906	-26.98635	90.82631	B1	34	0.00000
1178	116	GLN	CG	-31.33401	-27.96419	89.80983	B1	34	0.00000
1179	116	GLN	CD	-31.33954	-27.31473	88.43588	B1	34	0.00000
1180	116	GLN	OE1	-32.32002	-27.33002	87.70605	B1	34	0.00000
1181	116	GLN	NE2	-30.20428	-26.71450	88.08185	B1	34	0.00000
1182	116	GLN	HE21	-29.39553	-26.71396	88.67007	B1	34	0.00000
1183	116	GLN	HE22	-30.15594	-26.24641	87.20205	B1	34	0.00000
1184	116	GLN	C	-29.89899	-28.73663	92.53043	B1	34	0.00000
1185	116	GLN	O	-30.38571	-29.77893	92.10767	B1	34	0.00000
1186	117	GLU	N	-28.76921	-28.72803	93.24838	B1	35	0.00000
1187	117	GLU	H	-28.34990	-27.88576	93.59525	B1	35	0.00000
1188	117	GLU	CA	-28.17324	-30.02538	93.58636	B1	35	0.00000
1189	117	GLU	CB	-26.68237	-30.02385	93.23572	B1	35	0.00000
1190	117	GLU	CG	-26.41125	-29.71932	91.75724	B1	35	0.00000
1191	117	GLU	CD	-24.93459	-29.87167	91.43636	B1	35	0.00000
1192	117	GLU	OE1	-24.62388	-30.40776	90.37359	B1	35	0.00000
1193	117	GLU	OE2	-24.09945	-29.45965	92.24135	B1	35	0.00000
1194	117	GLU	C	-28.34342	-30.39133	95.05360	B1	35	0.00000
1195	117	GLU	O	-28.39032	-29.54087	95.93593	B1	35	0.00000
1196	118	GLU	N	-28.45418	-31.70267	95.31151	B1	36	0.00000
1197	118	GLU	H	-28.37884	-32.37663	94.57856	B1	36	0.00000
1198	118	GLU	CA	-28.64640	-32.12718	96.70604	B1	36	0.00000
1199	118	GLU	CB	-28.86529	-33.64399	96.80220	B1	36	0.00000
1200	118	GLU	CG	-30.04821	-34.25904	96.04454	B1	36	0.00000
1201	118	GLU	CD	-30.18685	-35.73854	96.39969	B1	36	0.00000
1202	118	GLU	OE1	-31.31366	-36.18552	96.62004	B1	36	0.00000
1203	118	GLU	OE2	-29.17775	-36.44658	96.46236	B1	36	0.00000
1204	118	GLU	C	-27.45968	-31.79603	97.59954	B1	36	0.00000
1205	118	GLU	O	-26.30375	-31.93771	97.22004	B1	36	0.00000
1206	119	SER	N	-27.77719	-31.35385	98.81671	B1	37	0.00000
1207	119	SER	H	-28.73032	-31.22468	99.10568	B1	37	0.00000
1208	119	SER	CA	-26.67523	-31.09310	99.74333	B1	37	0.00000
1209	119	SER	CB	-26.79679	-29.64425	100.25438	B1	37	0.00000
1210	119	SER	OG	-25.62406	-29.23340	100.96654	B1	37	0.00000
1211	119	SER	HG	-25.73840	-28.33730	101.30354	B1	37	0.00000
1212	119	SER	C	-26.64967	-32.10869	100.87899	B1	37	0.00000

FIG. 20

./DR1_MIN2.CRD Thu Feb 25 14:58:48 1993 20

1213	119	SER	O	25.72568	-32.90554	101.03211	B1	37	0.00000
1214	120	VAL	N	-27.72434	-32.06808	101.67561	B1	38	0.00000
1215	120	VAL	H	-28.50026	-31.45938	101.48344	B1	38	0.00000
1216	120	VAL	CA	-27.82678	-32.99802	102.80099	B1	38	0.00000
1217	120	VAL	CB	-27.44790	-32.32244	104.13888	B1	38	0.00000
1218	120	VAL	CG1	-25.93252	-32.18078	104.29388	B1	38	0.00000
1219	120	VAL	CG2	-28.15631	-30.97900	104.33500	B1	38	0.00000
1220	120	VAL	C	-29.23777	-33.53625	102.89372	B1	38	0.00000
1221	120	VAL	O	-30.19812	-32.88656	102.49711	B1	38	0.00000
1222	121	ARG	N	-29.34164	-34.75356	103.41944	B1	39	0.00000
1223	121	ARG	H	-28.52525	-35.27675	103.67737	B1	39	0.00000
1224	121	ARG	CA	-30.65941	-35.37282	103.49447	B1	39	0.00000
1225	121	ARG	CB	-30.83879	-36.26556	102.25451	B1	39	0.00000
1226	121	ARG	CG	-32.24891	-36.83907	102.13977	B1	39	0.00000
1227	121	ARG	CD	-32.36448	-38.11228	101.31436	B1	39	0.00000
1228	121	ARG	NE	-33.46636	-38.89614	101.86585	B1	39	0.00000
1229	121	ARG	HE	-33.58314	-38.82444	102.86363	B1	39	0.00000
1230	121	ARG	CZ	-34.21779	-39.71705	101.13259	B1	39	0.00000
1231	121	ARG	NH1	-35.18842	-40.40193	101.73316	B1	39	0.00000
1232	121	ARG	HH11	-35.77971	-41.03741	101.23780	B1	39	0.00000
1233	121	ARG	HH12	-35.33365	-40.28453	102.71808	B1	39	0.00000
1234	121	ARG	NH2	-33.99786	-39.84536	99.82444	B1	39	0.00000
1235	121	ARG	HH21	-34.53079	-40.47140	99.25675	B1	39	0.00000
1236	121	ARG	HH22	-33.27054	-39.30635	99.39731	B1	39	0.00000
1237	121	ARG	C	-30.80743	-36.21013	104.75602	B1	39	0.00000
1238	121	ARG	O	-29.86515	-36.82872	105.23483	B1	40	0.00000
1239	122	PHE	N	-32.04075	-36.24095	105.26404	B1	40	0.00000
1240	122	PHE	H	-32.75061	-35.63810	104.89111	B1	40	0.00000
1241	122	PHE	CA	-32.40668	-37.26064	106.24769	B1	40	0.00000
1242	122	PHE	CB	-33.75724	-36.87165	106.85296	B1	40	0.00000
1243	122	PHE	CG	-33.64992	-36.46831	108.30418	B1	40	0.00000
1244	122	PHE	CD1	-32.56100	-35.69712	108.77664	B1	40	0.00000
1245	122	PHE	CD2	-34.66985	-36.87929	109.19094	B1	40	0.00000
1246	122	PHE	CE1	-32.49275	-35.34303	110.14035	B1	40	0.00000
1247	122	PHE	CE2	-34.60187	-36.52254	110.55431	B1	40	0.00000
1248	122	PHE	CZ	-33.51285	-35.75823	111.02379	B1	40	0.00000
1249	122	PHE	C	-32.57844	-38.62424	105.60697	B1	40	0.00000
1250	122	PHE	O	-33.34168	-38.79208	104.65587	B1	41	0.00000
1251	123	ASP	N	-31.06201	-39.60796	106.15389	B1	41	0.00000
1252	123	ASP	H	-31.23184	-39.47015	106.92548	B1	41	0.00000
1253	123	ASP	CA	-32.08552	-40.93522	105.58825	B1	41	0.00000
1254	123	ASP	CB	-30.85171	-41.81726	105.76445	B1	41	0.00000
1255	123	ASP	CG	-29.93161	-41.56041	104.59405	B1	41	0.00000
1256	123	ASP	OD1	-28.81173	-41.11310	104.81757	B1	41	0.00000
1257	123	ASP	OD2	-30.34905	-41.80191	103.45856	B1	41	0.00000
1258	123	ASP	C	-33.32362	-41.63618	106.09965	B1	41	0.00000
1259	123	ASP	O	-34.00966	-41.21121	107.02319	B1	42	0.00000
1260	124	SER	N	-33.62443	-42.74250	105.41429	B1	42	0.00000
1261	124	SER	H	-32.95329	-43.10971	104.76900	B1	42	0.00000
1262	124	SER	CA	-34.94425	-43.35498	105.58880	B1	42	0.00000
1263	124	SER	CB	-35.18779	-44.37028	104.46149	B1	42	0.00000
1264	124	SER	OG	-36.57945	-44.70776	104.37671	B1	42	0.00000
1265	124	SER	HG	-36.91089	-44.87590	105.27413	B1	42	0.00000
1266	124	SER	C	-35.21640	-44.01057	106.93634	B1	42	0.00000
1267	124	SER	O	-36.33538	-44.42223	107.22372	B1	43	0.00000
1268	125	ASP	N	-34.16447	-44.10325	107.74330	B1	43	0.00000
1269	125	ASP	H	-33.26228	-43.73425	107.50494	B1	43	0.00000
1270	125	ASP	CA	-34.30492	-44.60689	109.10471	B1	43	0.00000
1271	125	ASP	CB	-32.96210	-45.24580	109.50620	B1	43	0.00000
1272	125	ASP	CG	-31.82155	-44.23245	109.55779	B1	43	0.00000
1273	125	ASP	OD1	-31.89194	-43.19553	108.89075	B1	43	0.00000
1274	125	ASP	OD2	-30.87249	-44.45676	110.29614	B1	43	0.00000
1275	125	ASP	C	-34.69374	-43.52244	110.10428	B1	43	0.00000
1276	125	ASP	O	-35.10540	-43.78461	111.22872	B1	43	0.00000

FIG. 21

./DR1_MIN2.CRD Thu Feb 25 14:58:48 1993 21

1277	126	VAL	N	- .51615	-42.26751	109.64790	B1	44	0.00000
1278	126	VAL	H	-34.20939	-42.12308	108.70456	B1	44	0.00000
1279	126	VAL	CA	-34.59346	-41.07914	110.50496	B1	44	0.00000
1280	126	VAL	CB	-36.04814	-40.82462	110.97592	B1	44	0.00000
1281	126	VAL	CG1	-36.22164	-39.41758	111.54094	B1	44	0.00000
1282	126	VAL	CG2	-37.04494	-41.00281	109.82481	B1	44	0.00000
1283	126	VAL	C	-33.57625	-41.13739	111.64961	B1	44	0.00000
1284	126	VAL	O	-33.78819	-40.75401	112.79533	B1	45	0.00000
1285	127	GLY	N	-32.41541	-41.66443	111.25324	B1	45	0.00000
1286	127	GLY	H	-32.31598	-42.01122	110.31755	B1	45	0.00000
1287	127	GLY	CA	-31.32244	-41.88201	112.19529	B1	45	0.00000
1288	127	GLY	C	-29.94594	-41.56889	111.62542	B1	45	0.00000
1289	127	GLY	O	-29.03055	-41.21776	112.35962	B1	46	0.00000
1290	128	GLU	N	-29.81143	-41.65704	110.29545	B1	46	0.00000
1291	128	GLU	H	-30.48653	-42.13586	109.72534	B1	46	0.00000
1292	128	GLU	CA	-28.56256	-41.14297	109.73120	B1	46	0.00000
1293	128	GLU	CB	-27.75197	-42.29481	109.11709	B1	46	0.00000
1294	128	GLU	CG	-26.29316	-42.25781	109.59860	B1	46	0.00000
1295	128	GLU	CD	-25.44181	-43.20422	108.87693	B1	46	0.00000
1296	128	GLU	OE1	-24.49646	-42.88073	108.19992	B1	46	0.00000
1297	128	GLU	OE2	-25.71010	-44.47773	109.00348	B1	46	0.00000
1298	128	GLU	C	-28.71376	-39.98012	108.75031	B1	46	0.00000
1299	128	GLU	O	-29.80604	-39.57375	108.35724	B1	47	0.00000
1300	129	TYR	N	-27.54735	-39.42619	108.38931	B1	47	0.00000
1301	129	TYR	H	-26.68498	-39.83420	108.68820	B1	47	0.00000
1302	129	TYR	CA	-27.50019	-38.29454	107.46434	B1	47	0.00000
1303	129	TYR	CB	-26.63842	-37.15326	108.01560	B1	47	0.00000
1304	129	TYR	CG	-27.30857	-36.34222	109.09443	B1	47	0.00000
1305	129	TYR	CD1	-26.67181	-36.21958	110.34811	B1	47	0.00000
1306	129	TYR	CE1	-27.25566	-35.42131	111.35148	B1	47	0.00000
1307	129	TYR	CD2	-28.52827	-35.67832	108.83210	B1	47	0.00000
1308	129	TYR	CE2	-29.11235	-34.88063	109.83571	B1	47	0.00000
1309	129	TYR	CZ	-28.47327	-34.75726	111.08860	B1	47	0.00000
1310	129	TYR	OH	-29.05005	-33.98459	112.07221	B1	47	0.00000
1311	129	TYR	HH	-29.70394	-33.40059	111.67732	B1	47	0.00000
1312	129	TYR	C	-26.82531	-38.64384	106.15941	B1	47	0.00000
1313	129	TYR	O	-25.66697	-39.04407	106.10492	B1	48	0.00000
1314	130	ARG	N	-27.55686	-38.38162	105.08581	B1	48	0.00000
1315	130	ARG	H	-28.51666	-38.10451	105.16735	B1	48	0.00000
1316	130	ARG	CA	-26.87326	-38.41254	103.80227	B1	48	0.00000
1317	130	ARG	CB	-27.85650	-38.84699	102.71647	B1	48	0.00000
1318	130	ARG	CG	-27.21143	-39.00526	101.34112	B1	48	0.00000
1319	130	ARG	CD	-28.23975	-39.41974	100.29808	B1	48	0.00000
1320	130	ARG	NE	-27.66322	-39.38333	98.95629	B1	48	0.00000
1321	130	ARG	HE	-26.82589	-38.85034	98.82833	B1	48	0.00000
1322	130	ARG	CZ	-28.29934	-39.96348	97.93202	B1	48	0.00000
1323	130	ARG	NH1	-27.82365	-39.81313	96.69917	B1	48	0.00000
1324	130	ARG	HH11	-28.26738	-40.23513	95.90996	B1	48	0.00000
1325	130	ARG	HH12	-27.01064	-39.25297	96.53955	B1	48	0.00000
1326	130	ARG	NH2	-29.39843	-40.68730	98.14392	B1	48	0.00000
1327	130	ARG	HH21	-29.90446	-41.10492	97.39118	B1	48	0.00000
1328	130	ARG	HH22	-29.72741	-40.81930	99.07957	B1	48	0.00000
1329	130	ARG	C	-26.28084	-37.06053	103.45986	B1	48	0.00000
1330	130	ARG	O	-26.96293	-36.11772	103.07688	B1	49	0.00000
1331	131	ALA	N	-24.95816	-36.99899	103.58668	B1	49	0.00000
1332	131	ALA	H	-24.45069	-37.77908	103.95192	B1	49	0.00000
1333	131	ALA	CA	-24.28607	-35.84894	102.98902	B1	49	0.00000
1334	131	ALA	CB	-23.06137	-35.44271	103.80801	B1	49	0.00000
1335	131	ALA	C	-23.85084	-36.20633	101.58658	B1	49	0.00000
1336	131	ALA	O	-23.17892	-37.20632	101.36065	B1	50	0.00000
1337	132	VAL	N	-24.28495	-35.38774	100.63154	B1	50	0.00000
1338	132	VAL	H	-24.78984	-34.54695	100.85567	B1	50	0.00000
1339	132	VAL	CA	-24.05930	-35.79619	99.24192	B1	50	0.00000
1340	132	VAL	CB	-25.12578	-35.11200	98.36560	B1	50	0.00000

FIG. 22

./DR1_MIN2.CRD Thu Feb 25 14:58:48 1993 22

1341	132	VAL	CG1	5.02505	-35.45687	96.87606	B1	50	0.00000
1342	132	VAL	CG2	-6.51048	-35.48853	98.85777	B1	50	0.00000
1343	132	VAL	C	-22.64446	-35.53393	98.73419	B1	50	0.00000
1344	132	VAL	O	-22.12598	-36.19257	97.84114	B1	50	0.00000
1345	133	THR	N	-22.01646	-34.53567	99.35299	B1	51	0.00000
1346	133	THR	H	-22.44036	-34.04272	100.11190	B1	51	0.00000
1347	133	THR	CA	-20.68297	-34.13851	98.91128	B1	51	0.00000
1348	133	THR	CB	-20.84979	-33.09962	97.76600	B1	51	0.00000
1349	133	THR	OG1	-19.58519	-32.56706	97.34397	B1	51	0.00000
1350	133	THR	HG1	-19.69018	-32.10136	96.50551	B1	51	0.00000
1351	133	THR	CG2	-21.81730	-31.96947	98.12788	B1	51	0.00000
1352	133	THR	C	-19.91735	-33.59750	100.10846	B1	51	0.00000
1353	133	THR	O	-20.48697	-33.30952	101.15881	B1	51	0.00000
1354	134	GLU	N	-18.60119	-33.44216	99.91793	B1	52	0.00000
1355	134	GLU	H	-18.20352	-33.65725	99.02398	B1	52	0.00000
1356	134	GLU	CA	-17.75238	-32.88738	100.97647	B1	52	0.00000
1357	134	GLU	CB	-16.30452	-32.81284	100.49482	B1	52	0.00000
1358	134	GLU	CG	-15.76229	-34.17073	100.03844	B1	52	0.00000
1359	134	GLU	CD	-14.31377	-34.04410	99.60488	B1	52	0.00000
1360	134	GLU	OE1	-13.54341	-34.96158	99.88007	B1	52	0.00000
1361	134	GLU	OE2	-13.96021	-33.03519	98.99487	B1	52	0.00000
1362	134	GLU	C	-18.18601	-31.51310	101.45728	B1	52	0.00000
1363	134	GLU	O	-17.97884	-31.11916	102.59352	B1	52	0.00000
1364	135	LEU	N	-18.87611	-30.80674	100.55812	B1	53	0.00000
1365	135	LEU	H	-18.92762	-31.13340	99.61398	B1	53	0.00000
1366	135	LEU	CA	-19.55727	-29.57029	100.94931	B1	53	0.00000
1367	135	LEU	CB	-20.29914	-29.06218	99.70959	B1	53	0.00000
1368	135	LEU	CG	-20.12211	-27.57937	99.30843	B1	53	0.00000
1369	135	LEU	CD1	-20.93390	-26.68772	100.32666	B1	53	0.00000
1370	135	LEU	CD2	-18.63204	-27.23870	99.36436	B1	53	0.00000
1371	135	LEU	C	-20.53099	-29.72915	102.11412	B1	53	0.00000
1372	135	LEU	O	-20.60025	-28.93514	103.04463	B1	54	0.00000
1373	136	GLY	N	-21.29082	-30.82221	102.02891	B1	54	0.00000
1374	136	GLY	H	-21.14062	-31.49656	101.30480	B1	54	0.00000
1375	136	GLY	CA	-22.25373	-31.10000	103.08935	B1	54	0.00000
1376	136	GLY	C	-21.66227	-31.85099	104.26834	B1	54	0.00000
1377	136	GLY	O	-22.17280	-31.82013	105.38053	B1	55	0.00000
1378	137	ARG	N	-20.54192	-32.53644	104.01306	B1	55	0.00000
1379	137	ARG	H	-20.17033	-32.57514	103.08296	B1	55	0.00000
1380	137	ARG	CA	-19.94165	-33.32437	105.09532	B1	55	0.00000
1381	137	ARG	CB	-18.67070	-34.02762	104.58318	B1	55	0.00000
1382	137	ARG	CG	-18.13008	-35.07893	105.55025	B1	55	0.00000
1383	137	ARG	CD	-19.16855	-36.15719	105.85371	B1	55	0.00000
1384	137	ARG	NE	-18.66781	-37.06640	106.87657	B1	55	0.00000
1385	137	ARG	HE	-17.93002	-36.71980	107.47204	B1	55	0.00000
1386	137	ARG	CZ	-19.21896	-38.26612	107.07006	B1	55	0.00000
1387	137	ARG	NH1	-18.67934	-39.07643	107.97489	B1	55	0.00000
1388	137	ARG	HH11	-19.03969	-39.99255	108.14749	B1	55	0.00000
1389	137	ARG	HH12	-17.88763	-38.75541	108.49972	B1	55	0.00000
1390	137	ARG	NH2	-20.29085	-38.64369	106.37214	B1	55	0.00000
1391	137	ARG	HH21	-20.72192	-39.53705	106.49834	B1	55	0.00000
1392	137	ARG	HH22	-20.68879	-38.01490	105.70437	B1	55	0.00000
1393	137	ARG	C	-19.76330	-32.65026	106.46929	B1	55	0.00000
1394	137	ARG	O	-20.33202	-33.13638	107.44172	B1	56	0.00000
1395	138	PRO	N	-19.03095	-31.51331	106.56277	B1	56	0.00000
1396	138	PRO	CD	-18.26903	-30.78028	105.55482	B1	56	0.00000
1397	138	PRO	CA	-18.92500	-30.86885	107.87839	B1	56	0.00000
1398	138	PRO	CB	-18.00966	-29.66775	107.61418	B1	56	0.00000
1399	138	PRO	CG	-17.22921	-30.01427	106.35389	B1	56	0.00000
1400	138	PRO	C	-20.24853	-30.39451	108.45452	B1	56	0.00000
1401	138	PRO	O	-20.38873	-30.20105	109.65243	B1	57	0.00000
1402	139	ASP	N	-21.22822	-30.19407	107.56513	B1	57	0.00000
1403	139	ASP	H	-21.12955	-30.45258	106.60295	B1	57	0.00000
1404	139	ASP	CA	-22.54445	-29.76374	108.02635	B1	57	0.00000

FIG. 23

./SR1_MD:2.CRD Thu Feb 25 14:58:48 1993 23

1405	139	ASP	CB	3.29481	-29.22794	106.80729	B1	57	0.00000
1406	139	ASP	CG	-24.50680	-28.44150	107.23406	B1	57	0.00000
1407	139	ASP	OD1	-24.33925	-27.25955	107.53698	B1	57	0.00000
1408	139	ASP	OD2	-25.59590	-29.00937	107.24891	B1	57	0.00000
1409	139	ASP	C	-23.29009	-30.90651	108.70646	B1	57	0.00000
1410	139	ASP	O	-23.84428	-30.79944	109.79628	B1	58	0.00000
1411	140	ALA	N	-23.18867	-32.06950	108.04975	B1	58	0.00000
1412	140	ALA	H	-22.77745	-32.09325	107.13514	B1	58	0.00000
1413	140	ALA	CA	-23.64141	-33.29863	108.70194	B1	58	0.00000
1414	140	ALA	CB	-23.39932	-34.51285	107.80148	B1	58	0.00000
1415	140	ALA	C	-22.96994	-33.52591	110.04660	B1	58	0.00000
1416	140	ALA	O	-23.61501	-33.62460	111.08086	B1	58	0.00000
1417	141	GLU	N	-21.63141	-33.53710	110.01537	B1	59	0.00000
1418	141	GLU	H	-21.14260	-33.44422	109.14251	B1	59	0.00000
1419	141	GLU	CA	-20.88131	-33.73045	111.26272	B1	59	0.00000
1420	141	GLU	CB	-19.38545	-33.75474	110.92637	B1	59	0.00000
1421	141	GLU	CG	-19.08157	-34.92155	109.97183	B1	59	0.00000
1422	141	GLU	CD	-17.65605	-34.91070	109.44677	B1	59	0.00000
1423	141	GLU	OE1	-17.21662	-35.95752	108.96182	B1	59	0.00000
1424	141	GLU	OE2	-16.99658	-33.87375	109.50288	B1	59	0.00000
1425	141	GLU	C	-21.20315	-32.72395	112.36696	B1	59	0.00000
1426	141	GLU	O	-21.35204	-33.05368	113.53869	B1	60	0.00000
1427	142	TYR	N	-21.39109	-31.47026	111.93865	B1	60	0.00000
1428	142	TYR	H	-21.16858	-31.22939	110.99159	B1	60	0.00000
1429	142	TYR	CA	-21.91640	-30.42572	112.82625	B1	60	0.00000
1430	142	TYR	CB	-22.17510	-29.18770	111.95478	B1	60	0.00000
1431	142	TYR	CG	-22.15441	-27.86866	112.68902	B1	60	0.00000
1432	142	TYR	CD1	-20.91930	-27.21121	112.08286	B1	60	0.00000
1433	142	TYR	CE1	-20.89216	-25.94177	113.49633	B1	60	0.00000
1434	142	TYR	CD2	-23.36373	-27.27306	113.11310	B1	60	0.00000
1435	142	TYR	CE2	-23.33600	-26.00211	113.72688	B1	60	0.00000
1436	142	TYR	CZ	-22.10013	-25.34007	113.91274	B1	60	0.00000
1437	142	TYR	OH	-22.06472	-24.08718	114.49226	B1	60	0.00000
1438	142	TYR	HH	-22.95958	-23.75980	114.62492	B1	60	0.00000
1439	142	TYR	C	-23.20365	-30.84932	113.52485	B1	60	0.00000
1440	142	TYR	O	-23.33185	-30.86335	114.74427	B1	61	0.00000
1441	143	TRP	N	-24.16819	-31.24530	112.69102	B1	61	0.00000
1442	143	TRP	H	-24.01203	-31.27353	111.69669	B1	61	0.00000
1443	143	TRP	CA	-25.46084	-31.65772	113.24427	B1	61	0.00000
1444	143	TRP	CB	-26.46502	-31.82534	112.10045	B1	61	0.00000
1445	143	TRP	CG	-26.82927	-30.51319	111.43167	B1	61	0.00000
1446	143	TRP	CD2	-27.59514	-30.35383	110.26190	B1	61	0.00000
1447	143	TRP	CE2	-27.68725	-28.88192	110.01923	B1	61	0.00000
1448	143	TRP	CE3	-28.23171	-31.24445	109.37526	B1	61	0.00000
1449	143	TRP	CD1	-26.49404	-29.20408	111.84528	B1	61	0.00000
1450	143	TRP	NE1	-26.99373	-28.24161	111.01939	B1	61	0.00000
1451	143	TRP	HE1	-26.86335	-27.27405	111.09738	B1	61	0.00000
1452	143	TRP	CZ2	-28.41151	-28.41903	108.90296	B1	61	0.00000
1453	143	TRP	CZ3	-28.94655	-30.73482	108.27096	B1	61	0.00000
1454	143	TRP	CH2	-29.03488	-29.34388	108.03833	B1	61	0.00000
1455	143	TRP	C	-25.40824	-32.93379	114.07770	B1	61	0.00000
1456	143	TRP	O	-26.13451	-33.11650	115.04995	B1	62	0.00000
1457	144	ASN	N	-24.46546	-33.80055	113.69236	B1	62	0.00000
1458	144	ASN	H	-23.94027	-33.62305	112.85783	B1	62	0.00000
1459	144	ASN	CA	-24.16067	-34.99080	114.49069	B1	62	0.00000
1460	144	ASN	CB	-23.20850	-35.93308	113.73882	B1	62	0.00000
1461	144	ASN	CG	-23.89541	-36.68861	112.61740	B1	62	0.00000
1462	144	ASN	OD1	-23.68155	-36.47075	111.43371	B1	62	0.00000
1463	144	ASN	ND2	-24.72776	-37.64097	113.02365	B1	62	0.00000
1464	144	ASN	HD21	-24.89338	-37.81926	113.99276	B1	62	0.00000
1465	144	ASN	HD22	-25.19584	-38.20406	112.34455	B1	62	0.00000
1466	144	ASN	C	-23.49875	-34.69497	115.82591	B1	62	0.00000
1467	144	ASN	O	-23.43003	-35.54654	116.69924	B1	62	0.00000
1468	145	SER	N	-22.99604	-33.48640	115.97330	B1	63	0.00000

FIG. 24

1469	145	SER	H	22.97830	-32.80428	115.21961	B1	63	0.00000
1470	145	SER	CA	22.38004	-33.14621	117.25865	B1	63	0.00000
1471	145	SER	CB	-20.91921	-32.73054	117.01176	B1	63	0.00000
1472	145	SER	OG	-20.18983	-32.64180	118.24511	B1	63	0.00000
1473	145	SER	HG	-20.76055	-32.22535	118.91065	B1	63	0.00000
1474	145	SER	C	-23.11027	-32.07614	118.06161	B1	63	0.00000
1475	145	SER	O	-22.67401	-31.68287	119.13941	B1	63	0.00000
1476	146	GLN	N	-24.22180	-31.59037	117.51252	B1	64	0.00000
1477	146	GLN	H	-24.58118	-31.94604	116.64774	B1	64	0.00000
1478	146	GLN	CA	-24.90025	-30.49286	118.19522	B1	64	0.00000
1479	146	GLN	CB	-24.86315	-29.29301	117.23892	B1	64	0.00000
1480	146	GLN	CG	-25.45855	-27.96945	117.72882	B1	64	0.00000
1481	146	GLN	CD	-26.89096	-27.81462	117.25234	B1	64	0.00000
1482	146	GLN	OE1	-27.80837	-27.53609	118.00911	B1	64	0.00000
1483	146	GLN	NE2	-27.06556	-27.97948	115.94329	B1	64	0.00000
1484	146	GLN	HE21	-26.30809	-28.20349	115.33276	B1	64	0.00000
1485	146	GLN	HE22	-27.98288	-27.88997	115.56134	B1	64	0.00000
1486	146	GLN	C	-26.29488	-30.93694	118.57642	B1	64	0.00000
1487	146	GLN	O	-27.21649	-30.91839	117.77294	B1	64	0.00000
1488	147	LYS	N	-26.36947	-31.44426	119.82371	B1	65	0.00000
1489	147	LYS	H	-25.65249	-31.20699	120.47663	B1	65	0.00000
1490	147	LYS	CA	-27.35463	-32.46614	120.21964	B1	65	0.00000
1491	147	LYS	CB	-28.27258	-32.00851	121.37895	B1	65	0.00000
1492	147	LYS	CG	-29.34716	-33.02726	121.84203	B1	65	0.00000
1493	147	LYS	CD	-28.88674	-34.49172	121.97244	B1	65	0.00000
1494	147	LYS	CE	-29.96618	-35.46785	121.47444	B1	65	0.00000
1495	147	LYS	NZ	-29.40221	-36.81034	121.26907	B1	65	0.00000
1496	147	LYS	HZ1	-30.04886	-37.42223	120.71767	B1	65	0.00000
1497	147	LYS	HZ2	-28.53282	-36.76558	120.68922	B1	65	0.00000
1498	147	LYS	HZ3	-29.15199	-37.28892	122.15073	B1	65	0.00000
1499	147	LYS	C	-28.12445	-33.12689	119.09340	B1	65	0.00000
1500	147	LYS	O	-29.30235	-32.90174	118.83683	B1	65	0.00000
1501	148	ASP	N	-27.34620	-34.00916	118.45822	B1	66	0.00000
1502	148	ASP	H	-26.39747	-34.14495	118.75300	B1	66	0.00000
1503	148	ASP	CA	-27.79510	-35.00236	117.48362	B1	66	0.00000
1504	148	ASP	CB	-27.88927	-36.37833	118.17059	B1	66	0.00000
1505	148	ASP	CG	-26.79528	-36.57930	119.21585	B1	66	0.00000
1506	148	ASP	OD1	-25.69280	-36.06325	119.05193	B1	66	0.00000
1507	148	ASP	OD2	-27.07650	-37.20742	120.23524	B1	66	0.00000
1508	148	ASP	C	-29.08887	-34.63043	116.79645	B1	66	0.00000
1509	148	ASP	O	-30.17136	-35.14808	117.04951	B1	67	0.00000
1510	149	LEU	N	-28.92399	-33.61840	115.93941	B1	67	0.00000
1511	149	LEU	H	-27.98965	-33.30949	115.73440	B1	67	0.00000
1512	149	LEU	CA	-30.07076	-32.84036	115.45008	B1	67	0.00000
1513	149	LEU	CB	-29.45399	-31.74267	114.57360	B1	67	0.00000
1514	149	LEU	CG	-30.29432	-30.58223	114.02475	B1	67	0.00000
1515	149	LEU	CD1	-30.85820	-30.92475	112.65290	B1	67	0.00000
1516	149	LEU	CD2	-31.34761	-30.09615	115.02072	B1	67	0.00000
1517	149	LEU	C	-31.17667	-33.69413	114.80952	B1	67	0.00000
1518	149	LEU	O	-32.36472	-33.37859	114.83807	B1	68	0.00000
1519	150	LEU	N	-30.73118	-34.86138	114.32363	B1	68	0.00000
1520	150	LEU	H	-29.75579	-34.94139	114.11621	B1	68	0.00000
1521	150	LEU	CA	-31.59782	-36.02822	114.12850	B1	68	0.00000
1522	150	LEU	CB	-30.74740	-37.29867	114.15286	B1	68	0.00000
1523	150	LEU	CG	-29.89363	-37.44772	112.89569	B1	68	0.00000
1524	150	LEU	CD1	-20.64060	-38.26626	113.18796	B1	68	0.00000
1525	150	LEU	CD2	-30.71709	-38.01712	111.73915	B1	68	0.00000
1526	150	LEU	C	-32.74973	-36.17247	115.10785	B1	68	0.00000
1527	150	LEU	O	-33.89001	-36.01901	114.70350	B1	68	0.00000
1528	151	GLU	N	-32.47441	-36.43576	116.39428	B1	69	0.00000
1529	151	GLU	H	-31.52943	-36.57284	116.72119	B1	69	0.00000
1530	151	GLU	CA	-33.61295	-36.59512	117.30950	B1	69	0.00000
1531	151	GLU	CB	-33.19489	-36.98331	118.72928	B1	69	0.00000
1532	151	GLU	CG	-32.69081	-38.41906	118.86324	B1	69	0.00000

FIG. 25

./DK1_KLN2.CRD Thu Feb 25 14:58:48 1993 25

1533	151	GLU	CD	-31.19287	-38.44464	118.70497	B1	69	0.00000
1534	151	GLU	OE1	-30.71320	-38.33129	117.58148	B1	69	0.00000
1535	151	GLU	OE2	-30.51522	-38.56462	119.72459	B1	69	0.00000
1536	151	GLU	C	-34.55067	-35.41168	117.43857	B1	69	0.00000
1537	151	GLU	O	-35.75790	-35.57313	117.58647	B1	70	0.00000
1538	152	GLN	N	-33.98601	-34.19780	117.35586	B1	70	0.00000
1539	152	GLN	H	-33.00321	-34.10256	117.18602	B1	70	0.00000
1540	152	GLN	CA	-34.89656	-33.04752	117.40695	B1	70	0.00000
1541	152	GLN	CB	-34.15680	-31.71646	117.32018	B1	70	0.00000
1542	152	GLN	CG	-33.46159	-31.26900	118.60094	B1	70	0.00000
1543	152	GLN	CD	-33.23376	-29.77424	118.49387	B1	70	0.00000
1544	152	GLN	OE1	-32.13068	-29.27019	118.36008	B1	70	0.00000
1545	152	GLN	NE2	-34.34656	-29.04682	118.54711	B1	70	0.00000
1546	152	GLN	HE21	-35.24607	-29.46511	118.65663	B1	70	0.00000
1547	152	GLN	HE22	-34.28188	-28.05358	118.46911	B1	70	0.00000
1548	152	GLN	C	-35.89575	-33.04746	116.27182	B1	70	0.00000
1549	152	GLN	O	-37.09756	-32.85841	116.43607	B1	71	0.00000
1550	153	ARG	N	-35.34435	-33.30759	115.08552	B1	71	0.00000
1551	153	ARG	H	-34.35839	-33.48709	114.99299	B1	71	0.00000
1552	153	ARG	CA	-36.25853	-33.42129	113.95947	B1	71	0.00000
1553	153	ARG	CB	-35.46322	-33.43707	112.66564	B1	71	0.00000
1554	153	ARG	CG	-34.84280	-32.07791	112.35054	B1	71	0.00000
1555	153	ARG	CD	-33.88499	-32.22570	111.17839	B1	71	0.00000
1556	153	ARG	NE	-33.53171	-30.95306	110.55166	B1	71	0.00000
1557	153	ARG	HE	-33.79858	-30.09360	110.98860	B1	71	0.00000
1558	153	ARG	CZ	-33.01475	-31.01372	109.31716	B1	71	0.00000
1559	153	ARG	NH1	-32.97943	-29.92906	108.54980	B1	71	0.00000
1560	153	ARG	HH11	-32.81618	-30.04802	107.55422	B1	71	0.00000
1561	153	ARG	HH12	-33.14801	-29.01024	108.90136	B1	71	0.00000
1562	153	ARG	NH2	-32.57787	-32.17691	108.83735	B1	71	0.00000
1563	153	ARG	HH21	-32.40269	-32.29042	107.84355	B1	71	0.00000
1564	153	ARG	HH22	-32.45571	-32.97359	109.42307	B1	71	0.00000
1565	153	ARG	C	-37.16363	-34.62908	114.06926	B1	71	0.00000
1566	153	ARG	O	-38.37029	-34.50228	113.96948	B1	72	0.00000
1567	154	ARG	N	-36.57082	-35.79410	114.34589	B1	72	0.00000
1568	154	ARG	H	-35.57655	-35.83805	114.34685	B1	72	0.00000
1569	154	ARG	CA	-37.32441	-37.02834	114.59374	B1	72	0.00000
1570	154	ARG	CB	-36.30581	-38.11823	115.12926	B1	72	0.00000
1571	154	ARG	CG	-37.06240	-39.48786	115.22908	B1	72	0.00000
1572	154	ARG	CD	-36.14056	-40.61269	115.69023	B1	72	0.00000
1573	154	ARG	NE	-36.90866	-41.85162	115.80184	B1	72	0.00000
1574	154	ARG	HE	-37.59626	-42.01330	115.09038	B1	72	0.00000
1575	154	ARG	CZ	-36.70093	-42.71372	116.80504	B1	72	0.00000
1576	154	ARG	NH1	-37.45795	-43.80593	116.88687	B1	72	0.00000
1577	154	ARG	HH11	-37.33416	-44.47837	117.61587	B1	72	0.00000
1578	154	ARG	HH12	-38.17495	-43.96809	116.20728	B1	72	0.00000
1579	154	ARG	NH2	-35.75363	-42.48325	117.71513	B1	72	0.00000
1580	154	ARG	HH21	-35.59042	-43.10493	118.48012	B1	72	0.00000
1581	154	ARG	HH22	-35.18100	-41.66590	117.63709	B1	72	0.00000
1582	154	ARG	C	-38.52465	-36.88141	115.51516	B1	72	0.00000
1583	154	ARG	O	-39.58964	-37.43301	115.28503	B1	73	0.00000
1584	155	ARG	N	-38.35223	-36.06670	116.55472	B1	73	0.00000
1585	155	ARG	H	-37.44332	-35.69920	116.77047	B1	73	0.00000
1586	155	ARG	CA	-39.52250	-35.72569	117.36371	B1	73	0.00000
1587	155	ARG	CB	-39.05476	-34.79593	118.48265	B1	73	0.00000
1588	155	ARG	CG	-40.15723	-34.36970	119.44775	B1	73	0.00000
1589	155	ARG	CD	-39.62900	-33.36327	120.46128	B1	73	0.00000
1590	155	ARG	NE	-40.71623	-32.83780	121.28237	B1	73	0.00000
1591	155	ARG	HE	-41.63763	-33.18145	121.09517	B1	73	0.00000
1592	155	ARG	CZ	-40.47069	-31.92135	122.22743	B1	73	0.00000
1593	155	ARG	NH1	-41.48382	-31.43599	122.94081	B1	73	0.00000
1594	155	ARG	HH11	-41.33888	-30.75247	123.65592	B1	73	0.00000
1595	155	ARG	HH12	-42.41818	-31.75018	122.77039	B1	73	0.00000
1596	155	ARG	NH2	-39.22715	-31.49669	122.45304	B1	73	0.00000

FIG. 26

1661	162	ARG	NE	50.49694	-40.88455	114.11092	B1	80	0.00000
1662	162	ARG	CZ	49.34267	-42.40507	114.80601	B1	80	0.00000
1663	162	ARG	NH1	-50.23020	-43.32564	114.46730	B1	80	0.00000
1664	162	ARG	HH11	-50.11979	-44.31403	114.66150	B1	80	0.00000
1665	162	ARG	HH12	-51.06184	-43.06285	113.96028	B1	80	0.00000
1666	162	ARG	NH2	-48.19839	-42.76163	115.38323	B1	80	0.00000
1667	162	ARG	HH21	-48.00134	-43.72771	115.55650	B1	80	0.00000
1668	162	ARG	HH22	-47.52579	-42.06788	115.64161	B1	80	0.00000
1669	162	ARG	C	-49.75512	-35.92906	113.42487	B1	80	0.00000
1670	162	ARG	O	-50.82093	-35.93732	112.81658	B1	80	0.00000
1671	163	HIS	N	-49.58593	-35.31862	114.60088	B1	81	0.00000
1672	163	HIS	H	-48.68252	-35.28035	115.03933	B1	81	0.00000
1673	163	HIS	CA	-50.76431	-34.73357	115.23467	B1	81	0.00000
1674	163	HIS	CB	-50.42874	-34.29045	116.66134	B1	81	0.00000
1675	163	HIS	CG	-50.41026	-35.50649	117.55950	B1	81	0.00000
1676	163	HIS	ND1	-51.51644	-36.01842	118.12240	B1	81	0.00000
1677	163	HIS	HD1	-52.42830	-35.67431	118.03242	B1	81	0.00000
1678	163	HIS	CD2	-49.31404	-36.28837	117.93420	B1	81	0.00000
1679	163	HIS	NE2	-49.78030	-37.28089	118.73130	B1	81	0.00000
1680	163	HIS	CE1	-51.13423	-37.11585	118.84798	B1	81	0.00000
1681	163	HIS	C	-51.37160	-33.59588	114.44466	B1	81	0.00000
1682	163	HIS	O	-52.56947	-33.55956	114.18659	B1	81	0.00000
1683	164	ASN	N	-50.50246	-32.67616	114.01202	B1	82	0.00000
1684	164	ASN	H	-49.51981	-32.74462	114.21247	B1	82	0.00000
1685	164	ASN	CA	-51.04300	-31.58239	113.20331	B1	82	0.00000
1686	164	ASN	CB	-49.96583	-30.54361	112.89196	B1	82	0.00000
1687	164	ASN	CG	-49.91907	-29.53869	114.02377	B1	82	0.00000
1688	164	ASN	OD1	-49.13948	-29.62233	114.96163	B1	82	0.00000
1689	164	ASN	ND2	-50.80473	-28.55321	113.91309	B1	82	0.00000
1690	164	ASN	HD21	-51.44311	-28.49843	113.14586	B1	82	0.00000
1691	164	ASN	HD22	-50.84210	-27.84178	114.61251	B1	82	0.00000
1692	164	ASN	C	-51.70674	-32.02333	111.91584	B1	82	0.00000
1693	164	ASN	O	-52.73418	-31.48682	111.51085	B1	82	0.00000
1694	165	TYR	N	-51.12326	-33.05626	111.29191	B1	83	0.00000
1695	165	TYR	H	-50.28201	-33.49370	111.62194	B1	83	0.00000
1696	165	TYR	CA	-51.81304	-33.54191	110.10401	B1	83	0.00000
1697	165	TYR	CB	-50.92781	-34.47239	109.25048	B1	83	0.00000
1698	165	TYR	CG	-51.39689	-34.50284	107.80317	B1	83	0.00000
1699	165	TYR	CD1	-52.18946	-33.44669	107.29137	B1	83	0.00000
1700	165	TYR	CE1	-52.63312	-33.47413	105.96126	B1	83	0.00000
1701	165	TYR	CD2	-51.04289	-35.58963	106.96903	B1	83	0.00000
1702	165	TYR	CE2	-51.48846	-35.61522	105.62740	B1	83	0.00000
1703	165	TYR	CZ	-52.28557	-34.55457	105.13440	B1	83	0.00000
1704	165	TYR	OH	-52.75931	-34.53152	103.84155	B1	83	0.00000
1705	165	TYR	HH	-52.13515	-34.97162	103.24416	B1	83	0.00000
1706	165	TYR	C	-53.16114	-34.17050	110.39688	B1	83	0.00000
1707	165	TYR	O	-54.17243	-33.75040	109.85354	B1	83	0.00000
1708	166	GLY	N	-53.16827	-35.13255	111.32677	B1	84	0.00000
1709	166	GLY	H	-52.30920	-35.44284	111.74443	B1	84	0.00000
1710	166	GLY	CA	-54.44388	-35.75931	111.69489	B1	84	0.00000
1711	166	GLY	C	-55.55421	-34.78683	112.08191	B1	84	0.00000
1712	166	GLY	O	-56.70058	-34.86763	111.64884	B1	84	0.00000
1713	167	VAL	N	-55.16433	-33.81049	112.90998	B1	85	0.00000
1714	167	VAL	H	-54.21931	-33.77699	113.25020	B1	85	0.00000
1715	167	VAL	CA	-56.14083	-32.77588	113.26808	B1	85	0.00000
1716	167	VAL	CB	-55.54422	-31.87200	114.36486	B1	85	0.00000
1717	167	VAL	CG1	-56.46931	-30.71890	114.75691	B1	85	0.00000
1718	167	VAL	CG2	-55.22649	-32.70528	115.60849	B1	85	0.00000
1719	167	VAL	C	-56.62003	-31.96437	112.06515	B1	85	0.00000
1720	167	VAL	O	-57.80658	-31.70971	111.87365	B1	85	0.00000
1721	168	GLY	N	-55.65605	-31.61592	111.20320	B1	86	0.00000
1722	168	GLY	H	-54.68827	-31.81924	111.38362	B1	86	0.00000
1723	168	GLY	CA	-56.04215	-30.96490	109.94972	B1	86	0.00000
1724	168	GLY	C	-57.02338	-31.77629	109.11607	B1	86	0.00000

FIG. 28

1725	168	GLY	O	58.02649	-31.28044	108.61617	B1	86	0.00000
1726	169	GLU	N	56.71134	-33.07169	109.00665	B1	87	0.00000
1727	169	GLU	H	-55.87921	-33.43085	109.43169	B1	87	0.00000
1728	169	GLU	CA	-57.59179	-34.00467	108.30469	B1	87	0.00000
1729	169	GLU	CB	-56.95070	-35.39155	108.28846	B1	87	0.00000
1730	169	GLU	CG	-55.67851	-35.40281	107.43481	B1	87	0.00000
1731	169	GLU	CD	-54.91259	-36.69049	107.65905	B1	87	0.00000
1732	169	GLU	OE1	-53.74095	-36.61342	108.02205	B1	87	0.00000
1733	169	GLU	OE2	-55.48540	-37.76250	107.47736	B1	87	0.00000
1734	169	GLU	C	-59.00151	-34.05273	108.86565	B1	87	0.00000
1735	169	GLU	O	-59.98966	-34.06690	108.14126	B1	87	0.00000
1736	170	SER	N	-59.06996	-33.99305	110.19884	B1	88	0.00000
1737	170	SER	H	-58.23138	-34.05998	110.74831	B1	88	0.00000
1738	170	SER	CA	-60.38255	-33.85094	110.83391	B1	88	0.00000
1739	170	SER	CB	-60.18950	-33.85581	112.35798	B1	88	0.00000
1740	170	SER	OG	-61.42043	-34.13237	113.03659	B1	88	0.00000
1741	170	SER	HG	-61.30877	-34.00943	113.98374	B1	88	0.00000
1742	170	SER	C	-61.16415	-32.61665	110.37646	B1	88	0.00000
1743	170	SER	O	-62.31497	-32.69150	109.96191	B1	88	0.00000
1744	171	PHE	N	-60.49231	-31.45621	110.41676	B1	89	0.00000
1745	171	PHE	H	-59.54601	-31.41832	110.75393	B1	89	0.00000
1746	171	PHE	CA	-61.19539	-30.24631	109.95663	B1	89	0.00000
1747	171	PHE	CB	-60.30793	-28.99941	110.10880	B1	89	0.00000
1748	171	PHE	CG	-59.94208	-28.68147	111.54294	B1	89	0.00000
1749	171	PHE	CD1	-58.59291	-28.39703	111.85413	B1	89	0.00000
1750	171	PHE	CD2	-60.93098	-28.63398	112.55491	B1	89	0.00000
1751	171	PHE	CE1	-58.23032	-28.06074	113.17656	B1	89	0.00000
1752	171	PHE	CE2	-60.56845	-28.29967	113.87858	B1	89	0.00000
1753	171	PHE	CZ	-59.21901	-28.01319	114.18527	B1	89	0.00000
1754	171	PHE	C	-61.62802	-30.29139	108.49502	B1	89	0.00000
1755	171	PHE	O	-62.68697	-29.84047	108.07691	B1	89	0.00000
1756	172	THR	N	-60.72520	-30.85206	107.69903	B1	90	0.00000
1757	172	THR	H	-59.91792	-31.29854	108.09636	B1	90	0.00000
1758	172	THR	CA	-60.04308	-30.66246	106.25599	B1	90	0.00000
1759	172	THR	CB	-59.41710	-30.70747	105.70165	B1	90	0.00000
1760	172	THR	OG1	-59.35292	-30.21143	104.36207	B1	90	0.00000
1761	172	THR	HG1	-60.15430	-30.48800	103.89285	B1	90	0.00000
1762	172	THR	CG2	-58.90262	-32.13906	105.74825	B1	90	0.00000
1763	172	THR	C	-61.71208	-31.64877	105.47987	B1	90	0.00000
1764	172	THR	O	-61.76078	-31.56505	104.25169	B1	90	0.00000
1765	173	VAL	N	-62.32957	-32.60764	106.19315	B1	91	0.00000
1766	173	VAL	H	-62.28706	-32.56397	107.19363	B1	91	0.00000
1767	173	VAL	CA	-62.87984	-33.81113	105.53718	B1	91	0.00000
1768	173	VAL	CB	-63.87967	-34.51911	106.47899	B1	91	0.00000
1769	173	VAL	CG1	-64.50006	-35.77324	105.85034	B1	91	0.00000
1770	173	VAL	CG2	-63.20452	-34.90248	107.79466	B1	91	0.00000
1771	173	VAL	C	-63.51710	-33.59419	104.16716	B1	91	0.00000
1772	173	VAL	O	-63.18750	-34.24452	103.18126	B1	91	0.00000
1773	174	GLN	N	-64.41211	-32.59570	104.14711	B1	92	0.00000
1774	174	GLN	H	-64.59818	-32.11269	105.00138	B1	92	0.00000
1775	174	GLN	CA	-65.14373	-32.19104	102.94243	B1	92	0.00000
1776	174	GLN	CB	-65.76132	-30.80951	103.22574	B1	92	0.00000
1777	174	GLN	CG	-66.77986	-30.26016	102.21318	B1	92	0.00000
1778	174	GLN	CD	-66.09397	-29.58024	101.04012	B1	92	0.00000
1779	174	GLN	OE1	-65.45924	-28.54065	101.15380	B1	92	0.00000
1780	174	GLN	NE2	-66.26402	-30.18961	99.87453	B1	92	0.00000
1781	174	GLN	HE21	-66.63226	-31.11966	99.82928	B1	92	0.00000
1782	174	GLN	HE22	-65.97833	-29.74839	99.02730	B1	92	0.00000
1783	174	GLN	C	-64.36067	-32.18074	101.63553	B1	92	0.00000
1784	174	GLN	O	-64.88582	-32.51356	100.57991	B1	93	0.00000
1785	175	ARG	N	-63.09233	-31.77447	101.73327	B1	93	0.00000
1786	175	ARG	H	-62.69754	-31.53564	102.62225	B1	93	0.00000
1787	175	ARG	CA	-62.31707	-31.78835	100.50018	B1	93	0.00000
1788	175	ARG	CB	-61.85817	-30.36631	100.16958	B1	93	0.00000

FIG. 29

1789	175	ARG	CG	-61.24395	-30.26914	98.77310	B1	93	0.00000
1790	175	ARG	CD	-60.91597	-28.04209	98.34709	B1	93	0.00000
1791	175	ARG	NE	-59.98117	-28.87216	97.22615	B1	93	0.00000
1792	175	ARG	HE	-59.59146	-29.76910	97.00518	B1	93	0.00000
1793	175	ARG	CZ	-59.49795	-27.74924	96.68186	B1	93	0.00000
1794	175	ARG	NH1	-58.57343	-27.83579	95.72833	B1	93	0.00000
1795	175	ARG	HH11	-58.19414	-27.02728	95.28229	B1	93	0.00000
1796	175	ARG	HH12	-58.22480	-28.73459	95.46034	B1	93	0.00000
1797	175	ARG	NH2	-59.92427	-26.55682	97.09593	B1	93	0.00000
1798	175	ARG	HH21	-59.57028	-25.70796	96.70808	B1	93	0.00000
1799	175	ARG	HH22	-60.60311	-26.50975	97.82696	B1	93	0.00000
1800	175	ARG	C	-61.17336	-32.79150	100.46150	B1	93	0.00000
1801	175	ARG	O	-61.02327	-33.52738	99.49809	B1	93	0.00000
1802	176	ARG	N	-60.36493	-32.85103	101.53216	B1	94	0.00000
1803	176	ARG	H	-60.53761	-32.31340	102.35642	B1	94	0.00000
1804	176	ARG	CA	-59.25084	-33.80802	101.41499	B1	94	0.00000
1805	176	ARG	CB	-58.18750	-33.62483	102.49829	B1	94	0.00000
1806	176	ARG	CG	-57.32871	-32.37173	102.34974	B1	94	0.00000
1807	176	ARG	CD	-56.27515	-32.28237	103.45854	B1	94	0.00000
1808	176	ARG	NE	-56.30062	-30.94018	104.04511	B1	94	0.00000
1809	176	ARG	HE	-56.83150	-30.25818	103.53710	B1	94	0.00000
1810	176	ARG	CZ	-55.69078	-30.63659	105.19759	B1	94	0.00000
1811	176	ARG	NH1	-55.74431	-29.38340	105.64628	B1	94	0.00000
1812	176	ARG	HH11	-55.30471	-29.10955	106.50132	B1	94	0.00000
1813	176	ARG	HH12	-56.24080	-28.69008	105.12278	B1	94	0.00000
1814	176	ARG	NH2	-55.05038	-31.57276	105.89297	B1	94	0.00000
1815	176	ARG	HH21	-54.58912	-31.37726	106.75753	B1	94	0.00000
1816	176	ARG	HH22	-55.02183	-32.51329	105.54660	B1	94	0.00000
1817	176	ARG	C	-59.64686	-35.27348	101.42902	B1	94	0.00000
1818	176	ARG	O	-58.87808	-36.15316	101.06767	B1	94	0.00000
1819	177	VAL	N	-60.88626	-35.53390	101.85272	B1	95	0.00000
1820	177	VAL	H	-61.51901	-34.82991	102.18430	B1	95	0.00000
1821	177	VAL	CA	-61.32863	-36.91608	101.70299	B1	95	0.00000
1822	177	VAL	CB	-61.79519	-37.47193	103.06780	B1	95	0.00000
1823	177	VAL	CG1	-61.84113	-39.00335	103.05589	B1	95	0.00000
1824	177	VAL	CG2	-60.88761	-37.00753	104.21299	B1	95	0.00000
1825	177	VAL	C	-62.41412	-37.02458	100.63553	B1	95	0.00000
1826	177	VAL	O	-63.44404	-37.67295	100.79118	B1	95	0.00000
1827	178	HIS	N	-62.14889	-36.33028	99.52296	B1	96	0.00000
1828	178	HIS	H	-61.32158	-35.77698	99.39184	B1	96	0.00000
1829	178	HIS	CA	-63.09845	-36.32813	98.41659	B1	96	0.00000
1830	178	HIS	CB	-64.01495	-35.10064	98.57314	B1	96	0.00000
1831	178	HIS	CG	-65.27852	-35.21481	97.74669	B1	96	0.00000
1832	178	HIS	ND1	-65.30573	-35.62002	96.46944	B1	96	0.00000
1833	178	HIS	HD1	-64.50806	-35.91855	95.96816	B1	96	0.00000
1834	178	HIS	CD2	-66.58524	-34.92566	98.14872	B1	96	0.00000
1835	178	HIS	NE2	-67.39749	-35.16505	97.08780	B1	96	0.00000
1836	178	HIS	CE1	-66.60728	-35.59364	96.05191	B1	96	0.00000
1837	178	HIS	C	-62.34621	-36.29235	97.09131	B1	96	0.00000
1838	178	HIS	OCT1	-61.22615	-35.78756	97.07091	B1	96	0.00000
1839	178	HIS	OCT2	-62.87363	-36.77415	96.08759	B1	96	0.00000

FIG. 30

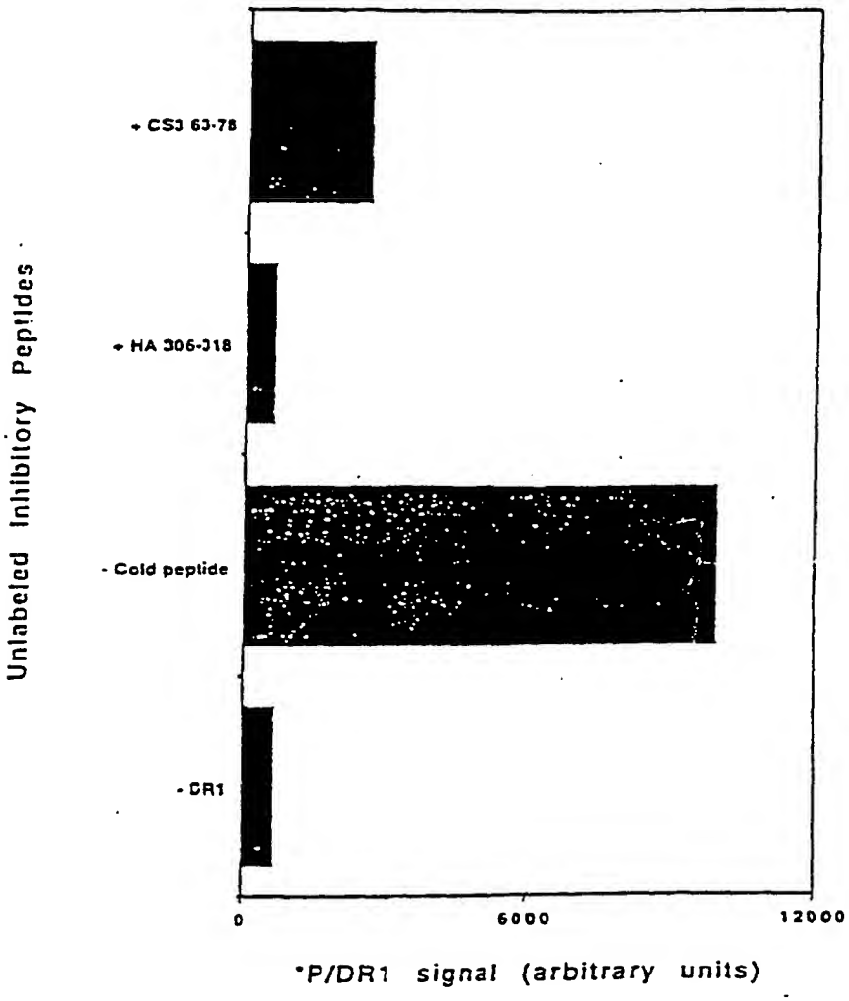
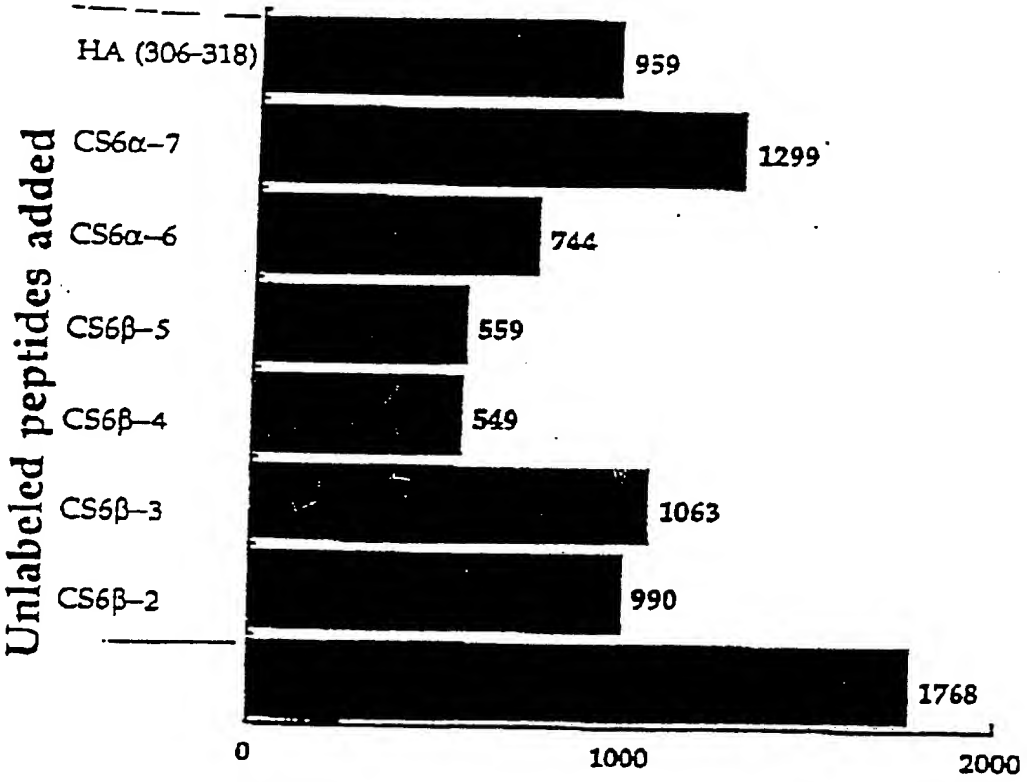

Unlabeled Inhibitory Peptides
+ CS3 63-75
+ HA 306-318
- Cold peptide
- DR1
0
6000
12000
*P/DR1 signal (arbitrary units)

FIG. 31

Inhibition of ^{125}I HA(306-318)/DR1 by unlabeled CS6 α and β peptides



*HA/DR1 compact dimer signal (densitometric units)

FIG. 32

INTERNATIONAL SEARCH REPORT

International application No.
PCT/US94/05697

A. CLASSIFICATION OF SUBJECT MATTER

IPC(5) :A61K 39/00, 39/02, 39/12, 37/02, 35/14
US CL :424/185.1, 186.1, 190.1, 242.1; 530/327, 326, 333, 334, 388.75
According to International Patent Classification (IPC) or to both national classification and IPC

B. FIELDS SEARCHED

Minimum documentation searched (classification system followed by classification symbols)

U.S. : 424/185.1, 186.1, 190.1, 242.1; 530/327, 326, 333, 334, 388.75

Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched

Electronic data base consulted during the international search (name of data base and, where practicable, search terms used)

C. DOCUMENTS CONSIDERED TO BE RELEVANT

Category*	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
X	The Journal of Immunology, Volume 150, No. 8, Part II, issued 15 April 1993, Nauss et al., " Binding Interactions of Peptides in a Structural Homology Model of the DR1 Class MHC ", page 41A, Abstract 221, see entire abstract.	1, 3-20
X ---- Y	Nature, Volume 358, issued 27 August 1992, Chicz et al., "Predominant Naturally Processed Peptides Bound to HLA-DR1 are derived from MHC-related Molecule and are Heterogenous in Size", pages 764-768, see page 766, Table 2, and Table 3.	12 ------ 1, 3-7

[X] Further documents are listed in the continuation of Box C. [ ] See patent family annex.

*	Special categories of cited documents:	"T"	later document published after the international filing date or priority date and not in conflict with the application but cited to understand the principle or theory underlying the invention
"A"	document defining the general state of the art which is not considered to be of particular relevance	"X"	document of particular relevance; the claimed invention cannot be considered novel or cannot be considered to involve an inventive step when the document is taken alone
"E"	earlier document published on or after the international filing date	"Y"	document of particular relevance; the claimed invention cannot be considered to involve an inventive step when the document is combined with one or more other such documents, such combination being obvious to a person skilled in the art
"L"	document which may throw doubts on priority claim(s) or which is cited to establish the publication date of another citation or other special reason (as specified)	"&"	document member of the same patent family
"O"	document referring to an oral disclosure, use, exhibition or other means		
"P"	document published prior to the international filing date but later than the priority date claimed		

Date of the actual completion of the international search 01 SEPTEMBER 1994	Date of mailing of the international search report 13 SEP 1994
Name and mailing address of the ISA/US Commissioner of Patents and Trademarks Box PCT Washington, D.C. 20231 Facsimile No. (703) 305-3230	Authorized officer H. Sidberry Telephone No. (703) 308-0196

Form PCT/ISA/210 (second sheet)(July 1992)*

INTERNATIONAL SEARCH REPORT

International application No.
PCT/US94/05697

C (Continuation). DOCUMENTS CONSIDERED TO BE RELEVANT

Category*	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
Y	The Journal of Immunology, Volume 150, No. 2, issued 15 January 1993, Boehncke et al., "The Importance of Dominant Negative Effects of Amino Acid Side Chain Substitution in Peptide-MHC Molecule Interactions and T Cell Recognition", pages 331-341, see Abstract, on page 331.	8-11
X	The EMBO Journal, Volume 9, No. 6, issued 1990, Jardetzky et al., "Peptide binding to HLA-DR1: a Peptide with most residues substituted to alanine retains MHC binding", pages 1797-1803, see page 1798, page 1800, figure 4, and page 1801, figure 7.	5--12
Y	Nature, Volume 332, issued 28 April 1988, Brown et al., "A hypothetical model of the foreign antigen binding site of Class II histocompatibility molecules", pages 845-850, see pages 845-849.	1, 3, 4

INTERNATIONAL SEARCH REPORT

International application No.
PCT/US94/05697

Box I Observations where certain claims were found unsearchable (Continuation of item 1 of first sheet)

This international report has not been established in respect of certain claims under Article 17(2)(a) for the following reasons:

1. [X] Claims Nos.: 2
because they relate to subject matter not required to be searched by this Authority, namely:

Claim 2 is directed to a computerized model which encompasses scientific theory and computer programs to the extent that the International Searching Authority is not equipped to search prior art concerning such programs. Accordingly claim 2 is withdrawn from search under PCT Rule 39 and PCT Article 17(2)(a)(i).

2. [ ] Claims Nos.:
because they relate to parts of the international application that do not comply with the prescribed requirements to such an extent that no meaningful international search can be carried out, specifically:

3. [ ] Claims Nos.:
because they are dependent claims and are not drafted in accordance with the second and third sentences of Rule 6.4(a).

Box II Observations where unity of invention is lacking (Continuation of item 2 of first sheet)

This International Searching Authority found multiple inventions in this international application, as follows:

1. [ ] As all required additional search fees were timely paid by the applicant, this international search report covers all searchable claims.

2. [ ] As all searchable claims could be searched without effort justifying an additional fee, this Authority did not invite payment of any additional fee.

3. [ ] As only some of the required additional search fees were timely paid by the applicant, this international search report covers only those claims for which fees were paid, specifically claims Nos.:

4. [ ] No required additional search fees were timely paid by the applicant. Consequently, this international search report is restricted to the invention first mentioned in the claims; it is covered by claims Nos.:

Remark n Protest

[ ] The additional search fees were accompanied by the applicant's protest.

[ ] No protest accompanied the payment f additional search fees.